

Grid-Enabled Adaptive Surrogate Modeling for Computer-Based Design

SUMO Lab

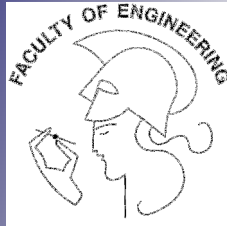
INTEC Broadband Communication Networks
Research Group (IBCN)

- Who are we ?
- Introduction
- Surrogate modeling
- SUMO Toolbox
- Examples
- Conclusions

- **Who are we ?**
 - who are we
 - what do we do
- **Introduction**
- **Surrogate modeling**
- **SUMO Toolbox**
- **Examples**
- **Conclusions**



Ghent University



Faculty of Engineering



Department of Information Technology
(INTEC)



INTEC Broadband and
Communications Networks (IBCN)





■ IBCN members

- 10 professors
- ~12 postdocs
- ~85 research members



■ SUMO Lab – (surrogate modeling)



■ Professor

- Tom Dhaene
- Eric Laermans

■ Postdoc

- Dirk Deschrijver

associated members (UA)

- Luciano De Tommasi

■ PhD students

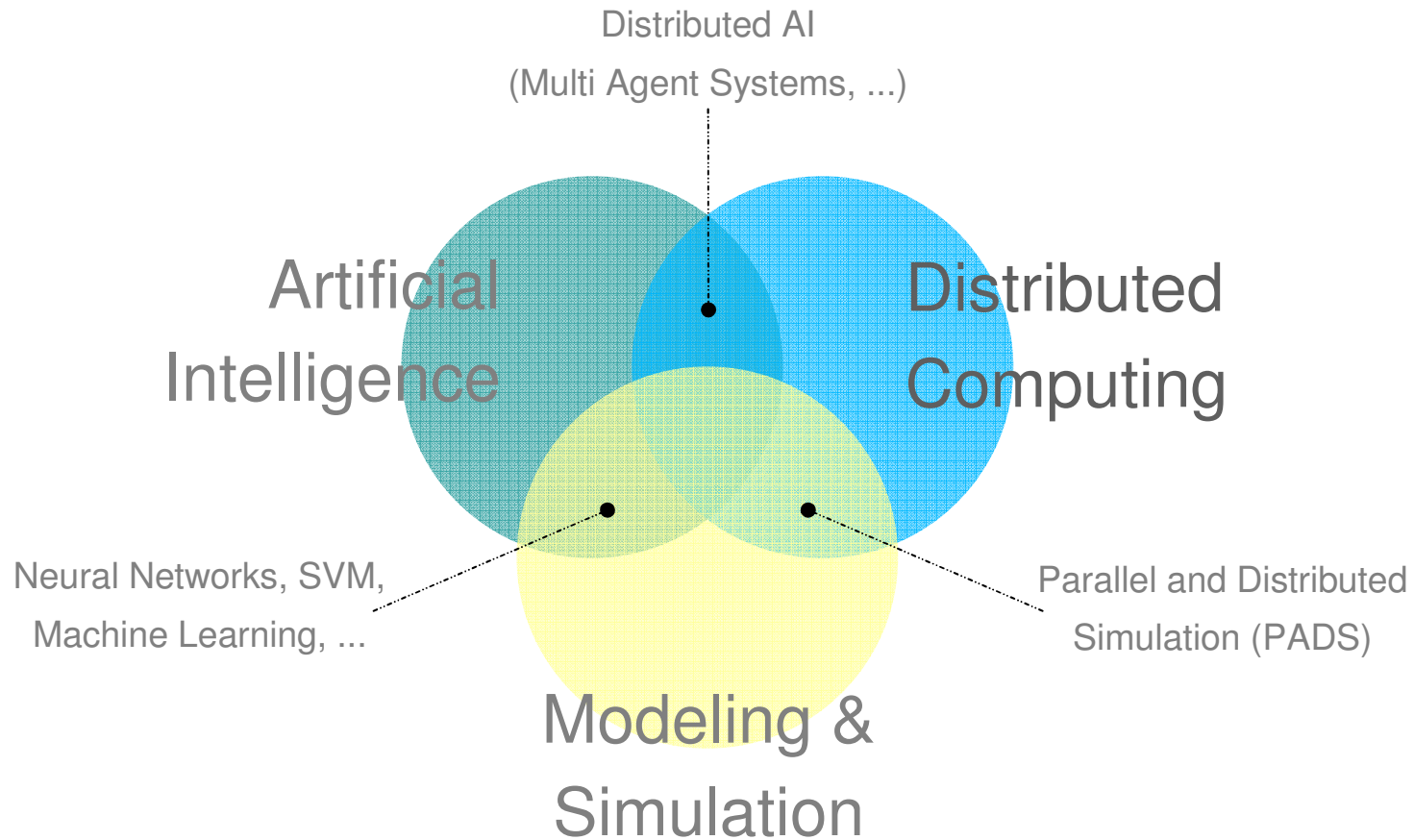
- Ivo Couckuyt
- Dirk Gorissen
- Francesco Ferranti
- Adam Narbudowicz

associated members (UA)

- Karel Crombecq
- Wouter Hendrickx

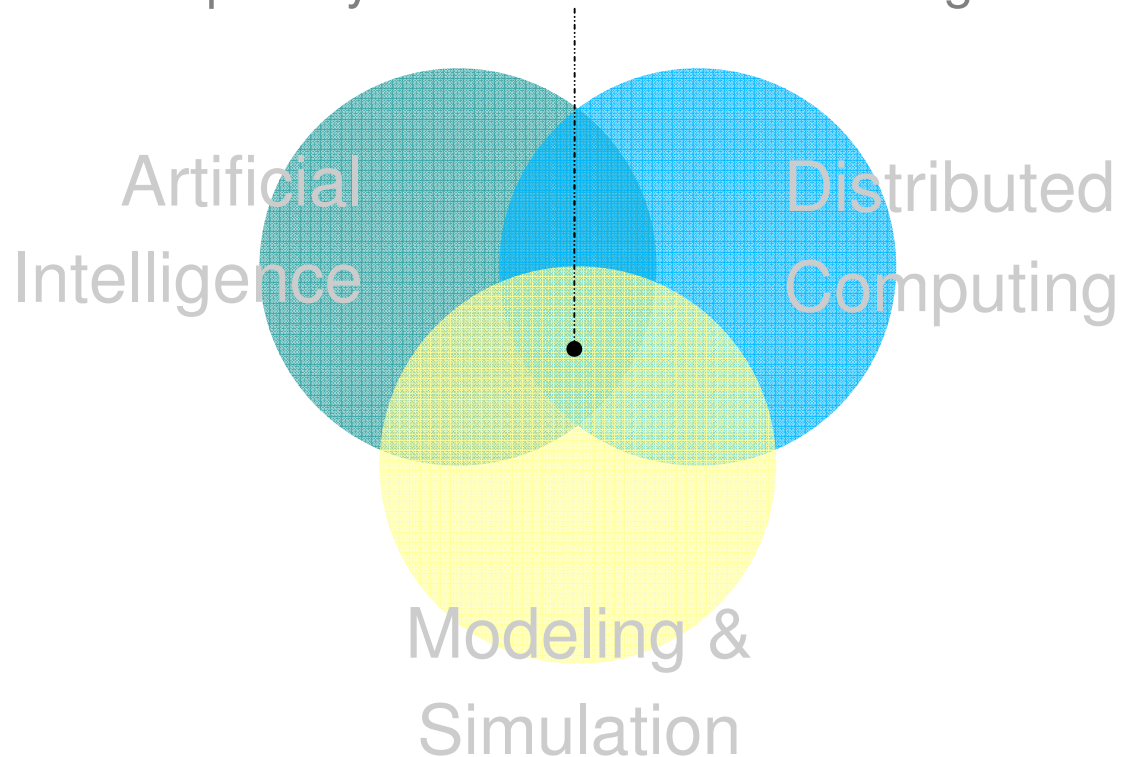
- **Surrogate models of complex systems**
 - replacement metamodels
- **Surrogate based optimization**
 - EGO based approaches
- **Machine learning and Experimental design**
- **High Performance Computing (HPC)**
- **(Parametric) Macromodels of electronic systems**
- **(Parametric) Model Order Reduction**

- **Surrogate models of complex systems**
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- (Parametric) Macromodels of electronic systems
- (Parametric) Model Order Reduction



Adaptive Surrogate Modeling

efficient and accurate characterization, modeling and simulation of complex systems in science and engineering



■ Who are we ?

■ Introduction

- Surrogate model ?
- What are we looking for ?
- Existing approaches and techniques

■ Surrogate modeling

■ SUMO Toolbox

■ Examples

■ Conclusions

- thousand years ago : **experimental science**
 - ♦ description of natural phenomena



- thousand years ago : **experimental science**
 - ♦ description of natural phenomena
- last few hundred years : **theoretical science**
 - ♦ Newton's laws, Maxwell's equations ...

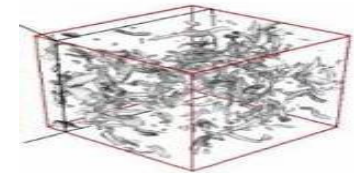


$$\frac{a}{a} = \frac{4\pi G\rho}{3} - \kappa \frac{c^2}{a^2}$$

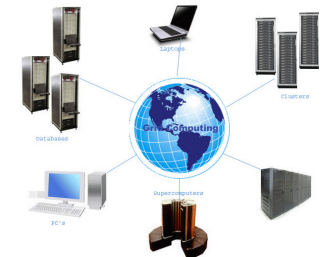
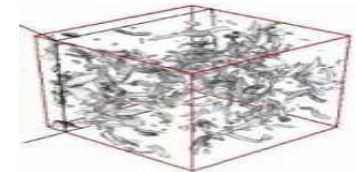
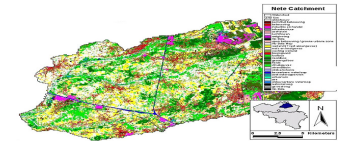
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- last few decades : **computational science**
 - ♦ simulation of complex phenomena



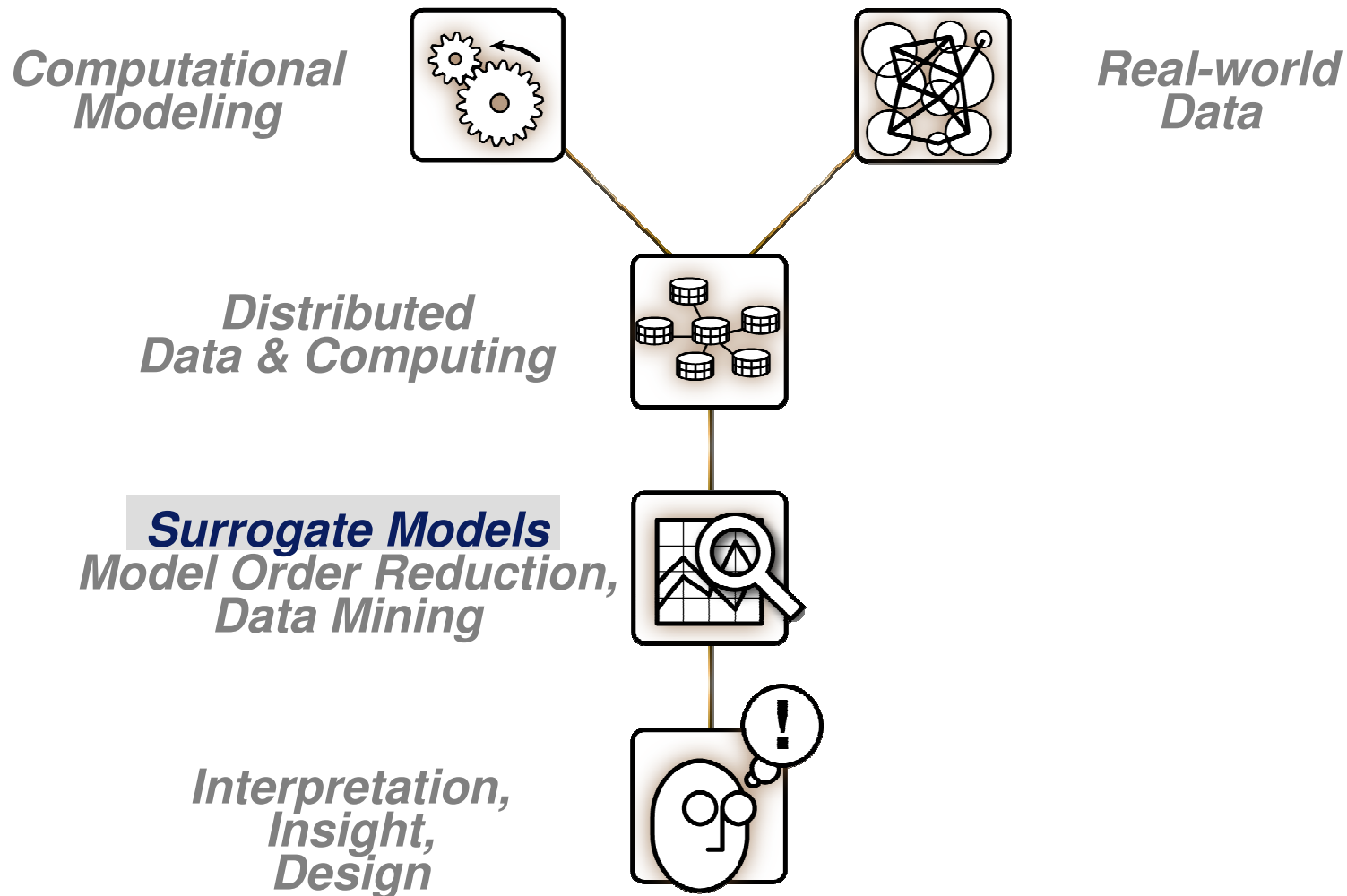
$$\left(\frac{a}{\alpha}\right)^2 = \frac{4\pi G\rho}{3} - \kappa \frac{c^2}{a^2}$$

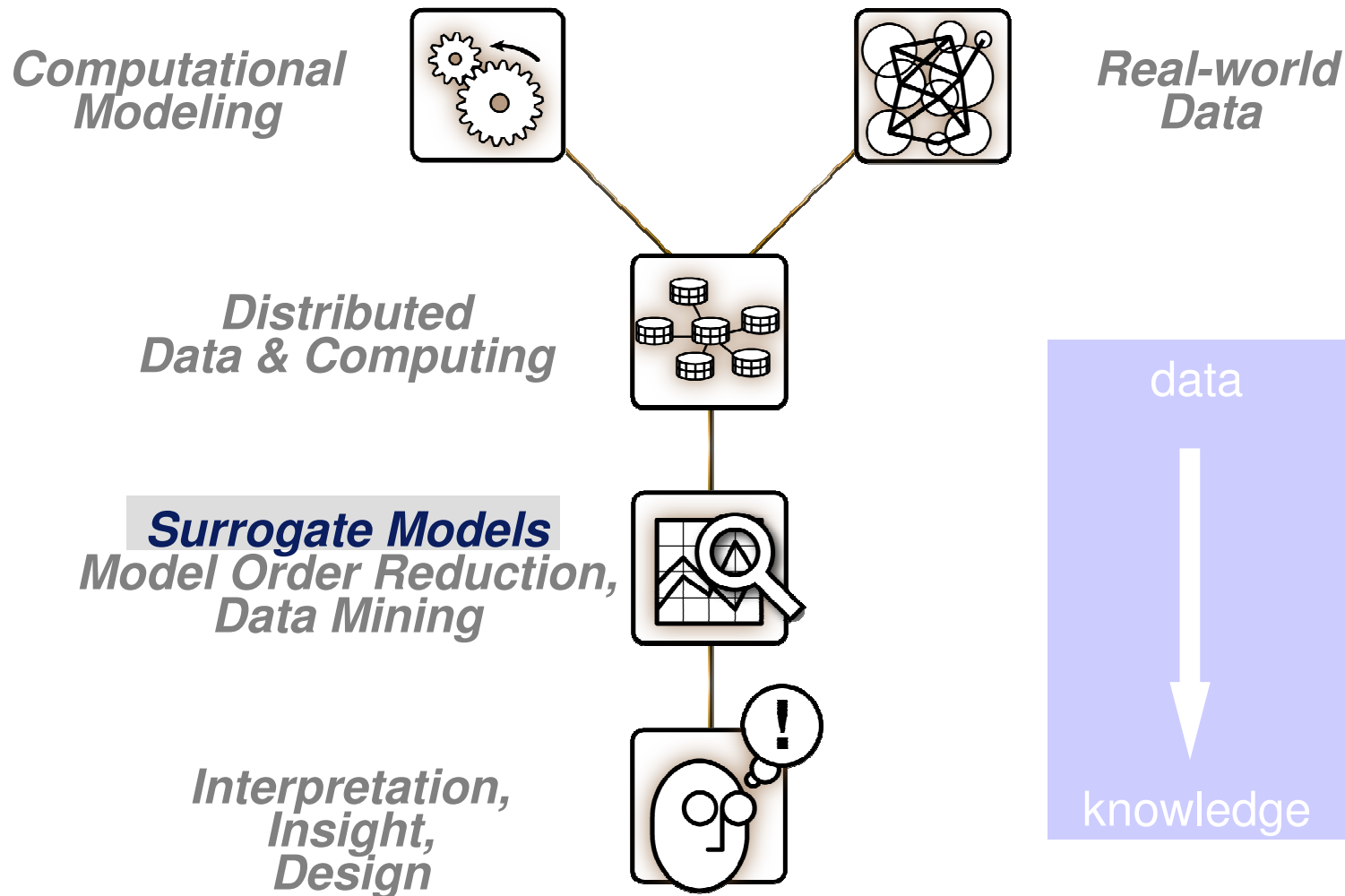


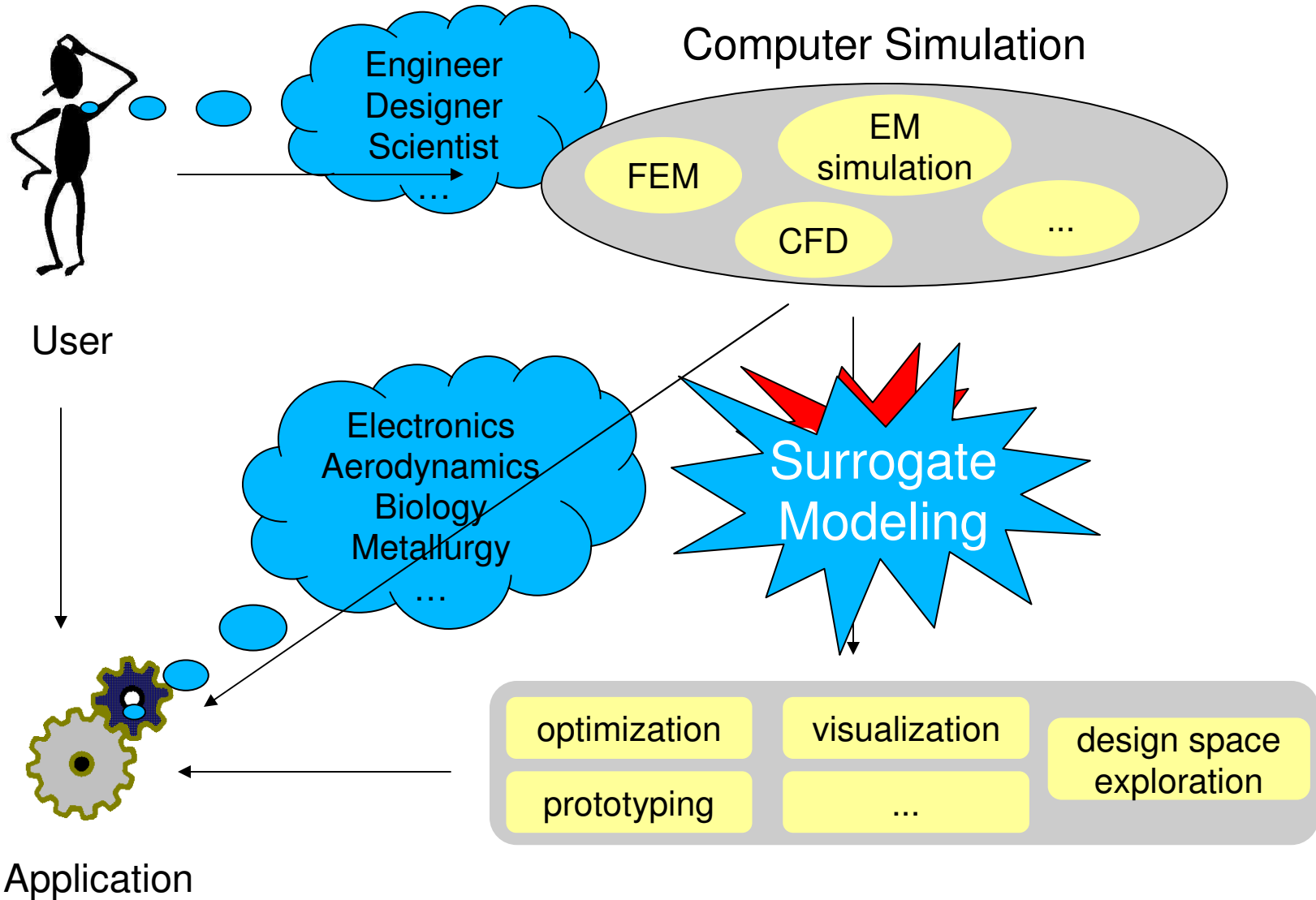
- thousand years ago : **experimental science**
 - ♦ description of natural phenomena
- last few hundred years : **theoretical science**
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- last few decades : **computational science**
 - ♦ simulation of complex phenomena
- today : **e-Science or data-centric science**
 - ♦ massive computing
 - ♦ large data exploration and mining
 - ♦ unify : theory, experiment, and simulation



(With thanks to Jim Gray)





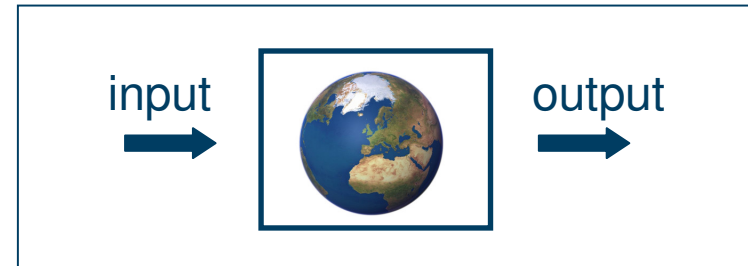


- **Surrogate modeling is not the only way**
 - Faster hardware, different approach, different solver, simplify problem (MOR, ...)
 - Right tool for the right job
- **Focus is on global surrogate modeling**
 - Though Surrogate Based Optimization (SBO) is not ignored either
- **Focus is on input-output problems**
 - Static, not dynamic
 - No time series prediction

■ system modeling

● real world

- ♦ I/O system
- ♦ stimulus / response



- ♦ examples: *mechanical, electrical, optical,
electronic, chemical ...
systems*

■ system modeling

- real world
 - ◆ I/O system
 - ◆ stimulus / response



- **simulation model**

- ◆ approximation
- ◆ discretization



- ◆ model = *abstraction of a real system*
- ◆ simulation = *virtual experiment*

■ system modeling

- real world
 - ◆ I/O system
 - ◆ stimulus / response
- simulation model
 - ◆ approximation
 - ◆ discretization
- **surrogate model**
 - ◆ metamodel, RSM, emulator
 - ◆ scalable analytical model
 - ◆ *“model of model”*



■ **simulation model** : widely used in engineering design

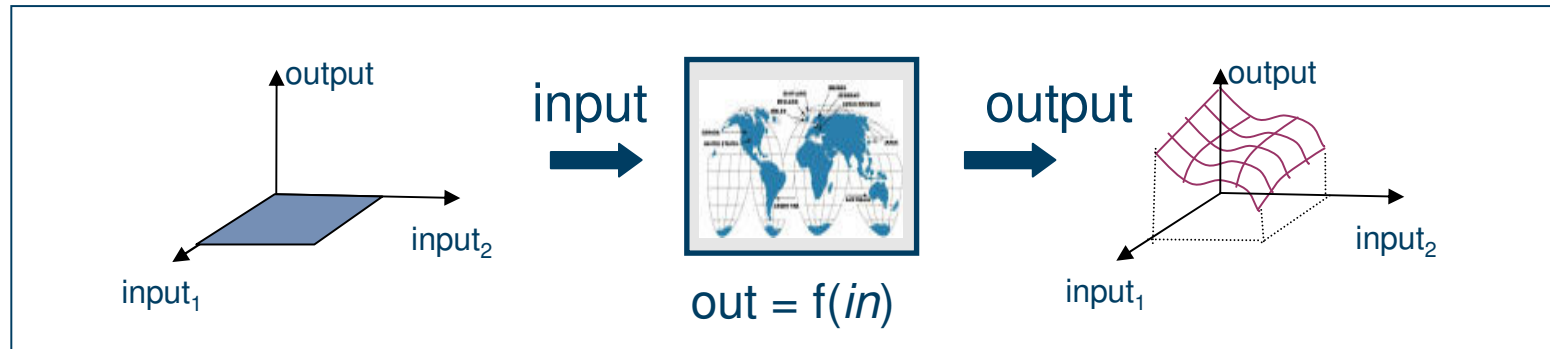


- each new sample in the input design space, requires new computer simulation
- accurate, high fidelity numerical model

■ however, simulation models...

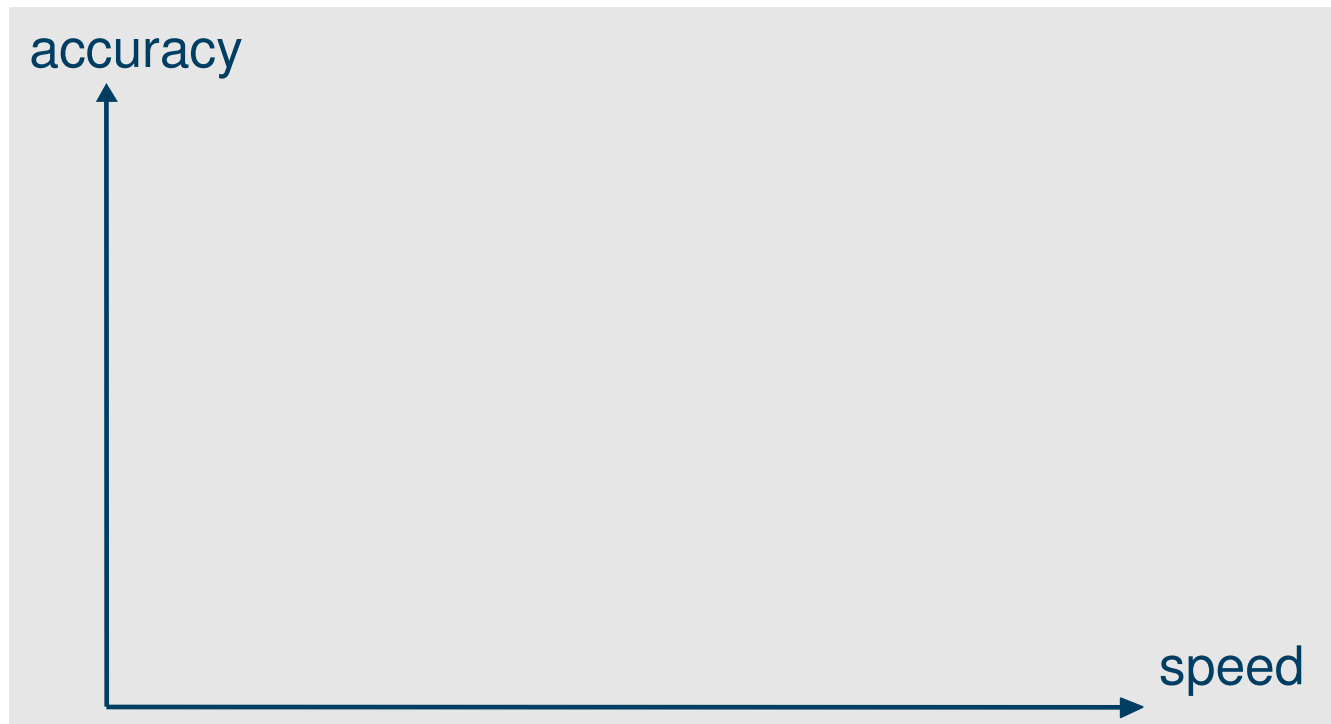
- ...complex
- ...time consuming to run
- ...optimization is expensive
- ...not always available
- ...highly specialized
 - ♦ **scalability?**
 - ♦ **model chaining?**
 - ♦ **integration with other tools?**
 - ♦ **hardware / software requirements?**
 - ♦ **licensing?**
 - ♦ ...

■ surrogate model



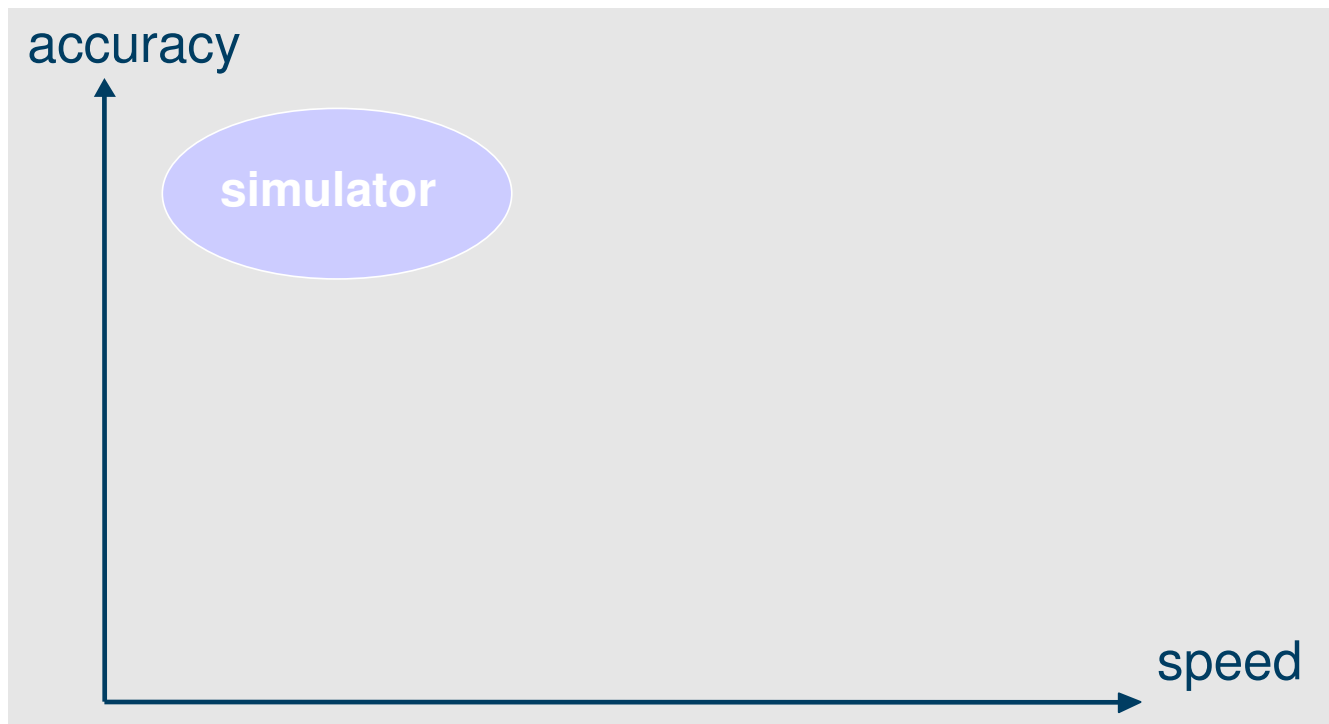
- analytical surrogate model
 - ◆ one-time upfront time investment
 - ◆ harness the power of the grid for simulation execution
 - ◆ adaptive sampling
- covers complete design space
 - ◆ design optimization, “*what-if*” analysis, sensitivity analysis

■ accuracy / speed trade-off



■ simulators

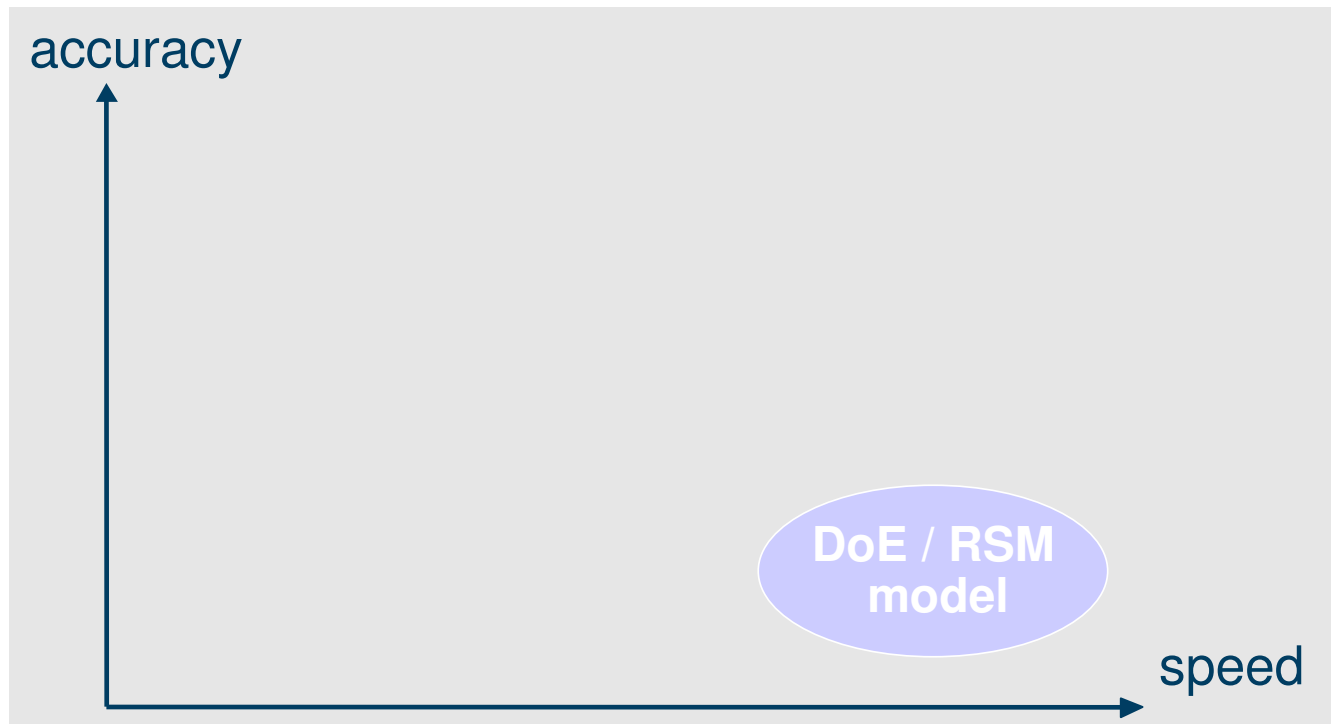
- domain-specific
- high-accuracy



■ models

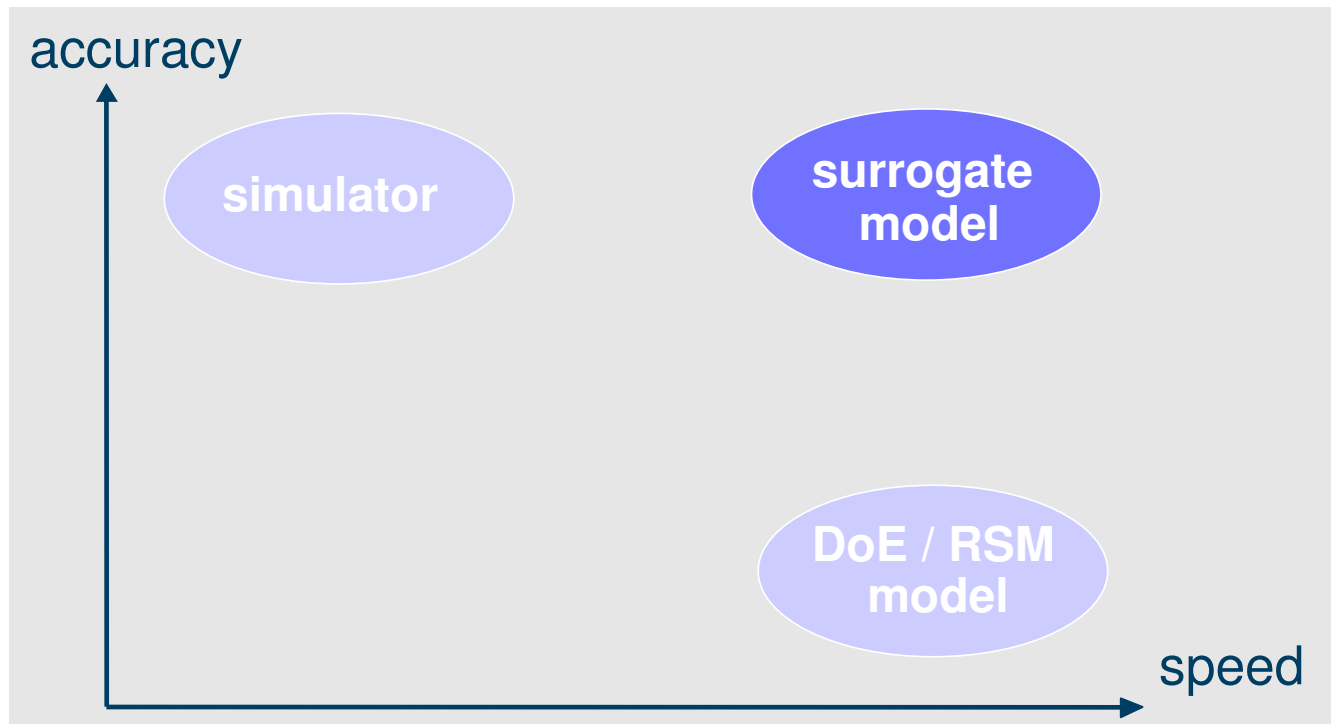
- 2nd order polynomial

Response Surface Models (RSM)



■ best of both worlds

- combining accuracy & generality of **simulators**, with the speed & flexibility of **models**



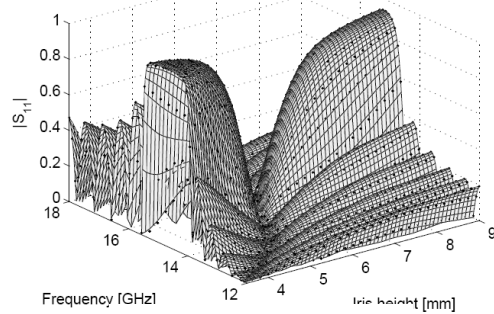
■ advantages

- instant evaluation
- compact formulation (few 100 parameters)

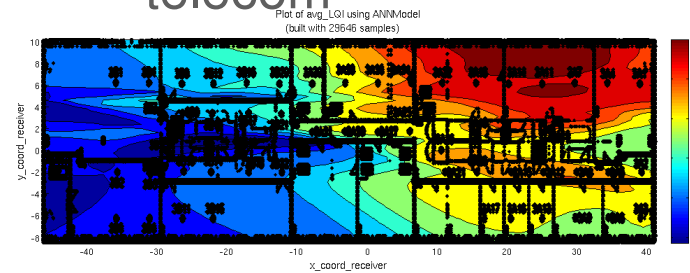
■ applications

- prototyping
- design space exploration
- design optimization
- sensitivity analysis
- *what-if* analysis
- ...

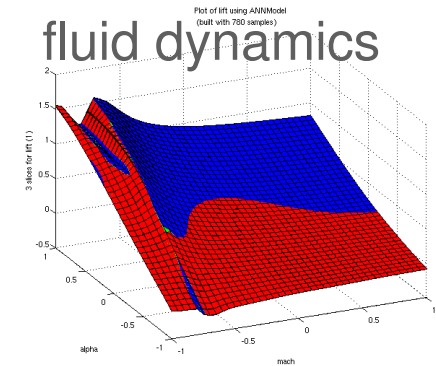
electronics



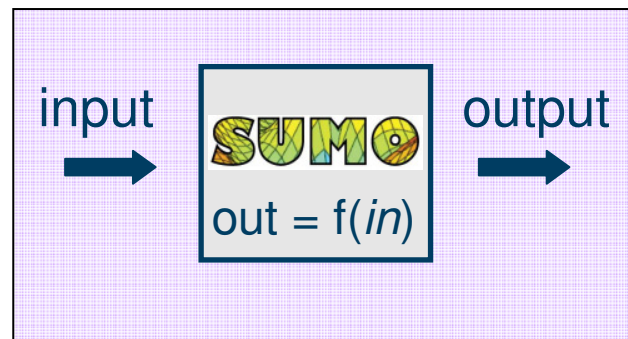
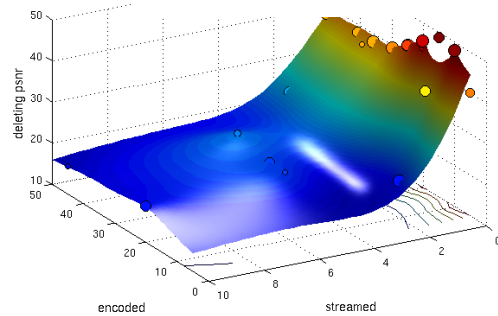
telecom



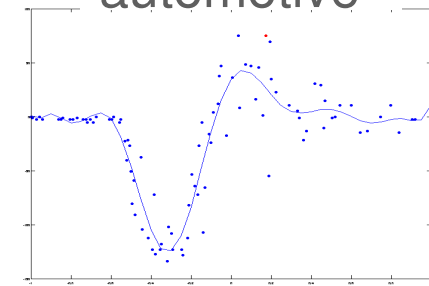
fluid dynamics



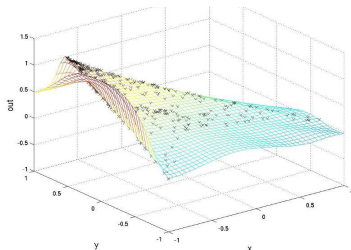
multimedia



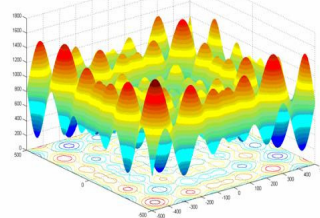
automotive



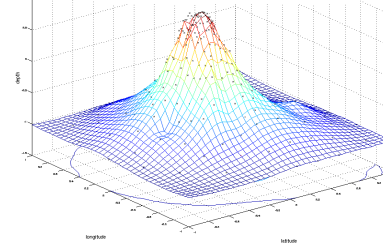
chemistry



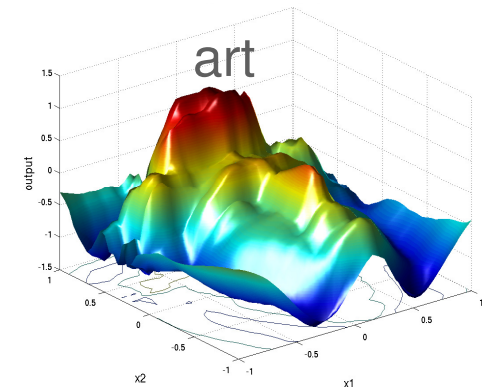
math



geology



art



■ challenges – research topics

- experimental design ?
- sample selection ?
- model selection, model tuning ?
 - type (e.g. *ANN, SVM, RBF, ...*)
 - complexity, hyperparameters (e.g. *#layers, #neurons* of ANN)
 - parameters (e.g. *weights* of ANN)
- black box – grey box – white box ?



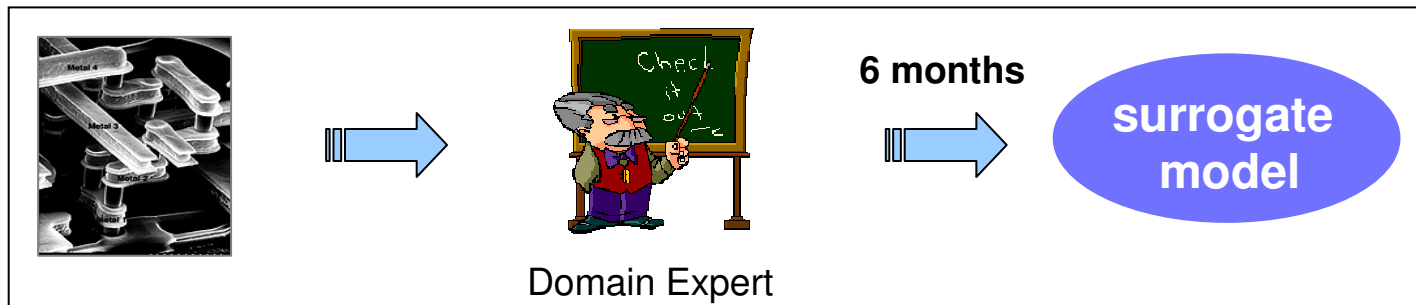
model assessment & selection crucial
only as good as data & designer

■ Grid-enabled adaptive algorithm for automatic surrogate model construction

- fully automated
- minimize prior, problem specific knowledge
 - ♦ **trade-off**
- minimal number of samples
 - ♦ **computationally expensive**
- support for distributed computing
- pre-defined accuracy
- pluggable / extensible
 - ♦ **no one-size-fits-all**
- integrate easily into the design process

■ traditional approaches

- discrete model library
 - ◆ database
- look-up tables, combined with local curve fitting
- hand-made analytical models
- ...



(With thanks to Luca Daniel (MIT))



■ common drawbacks

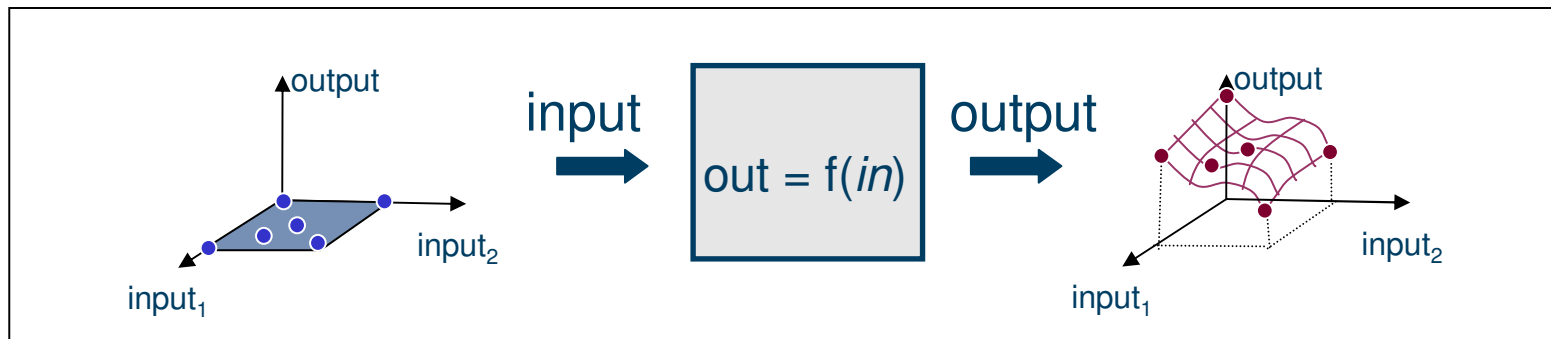
- oversampling / undersampling
 - ◆ waste of resources / important details missed
- overmodeling / undermodeling
- accuracy unknown
- prior knowledge required
- problem specific
- “*not invented here*” syndrome



highly skilled modeler
several months of work

- Who are we ?
- Introduction
- Surrogate modeling
 - adaptive modeling
 - adaptive sampling
 - distributed computing
 - adaptive surrogate modeling
- SUMO Toolbox
- Examples
- Conclusions

↪ scalable **surrogate model**, valid over design space

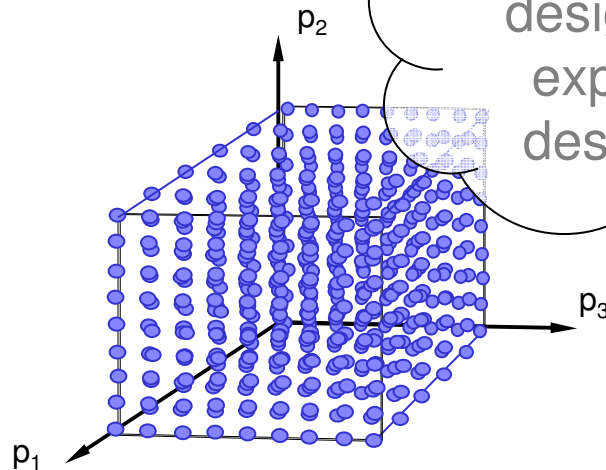


3 key technologies (+ 1 in development)

- ♦ adaptive data sampling
- ♦ adaptive model building
- ♦ distributed computing
- ♦ optimization

■ traditional approach

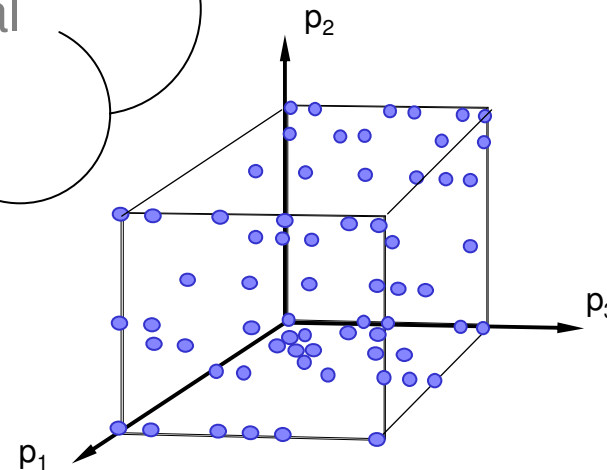
- uniform sampling
- oversampling
- undersampling



active learning,
sequential
design, optimal
experimental
design (OED)

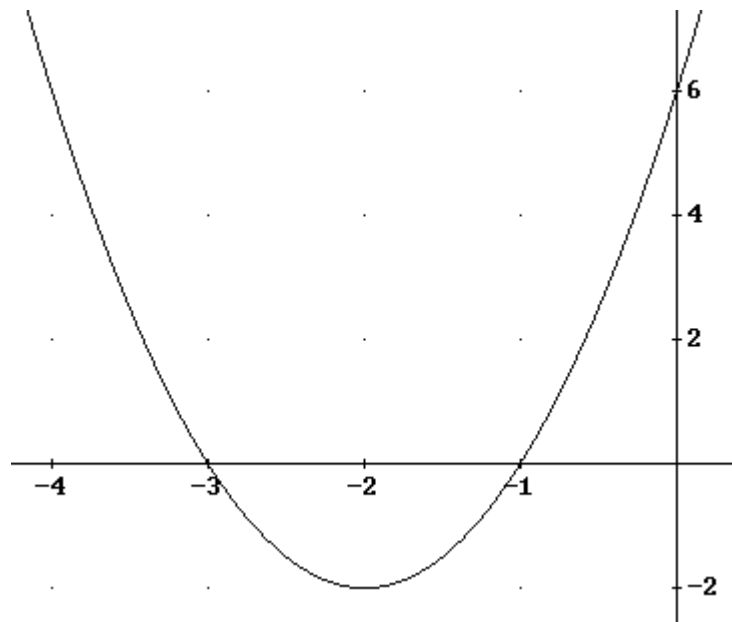
■ adaptive sampling

- “optimal” sample distribution
- *reflective exploration*



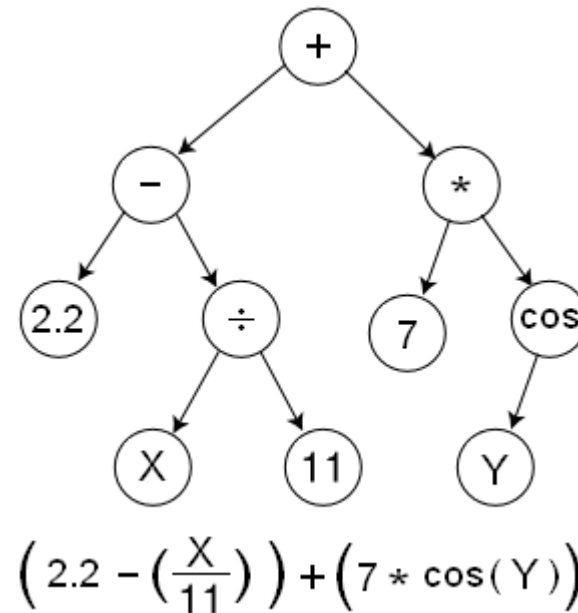
■ traditional approach

- local approximation
- overmodeling
- undermodeling



■ adaptive modeling

- global approximation
- optimal model complexity

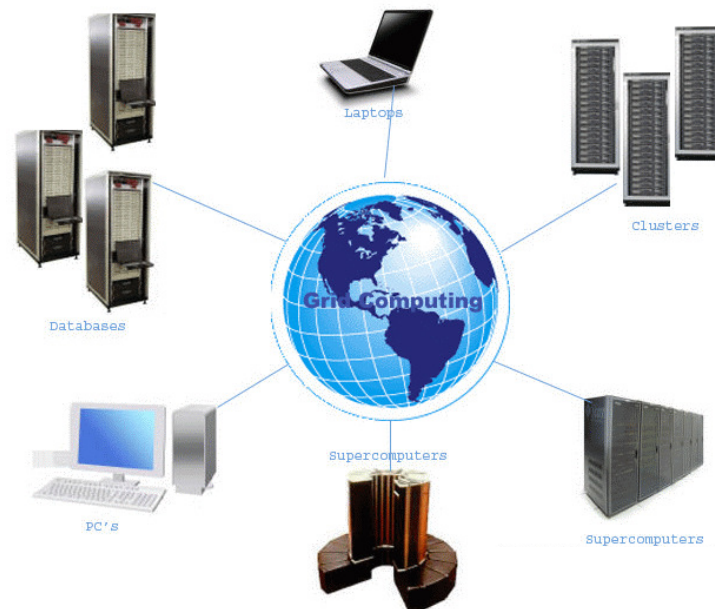


- traditional approach
 - sequential computing



■ distributed computing

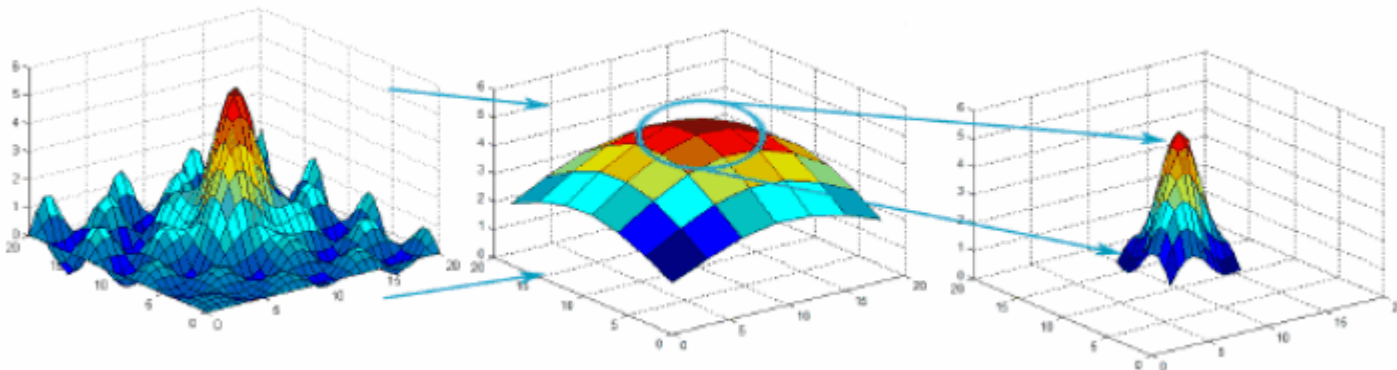
- cluster
- grid



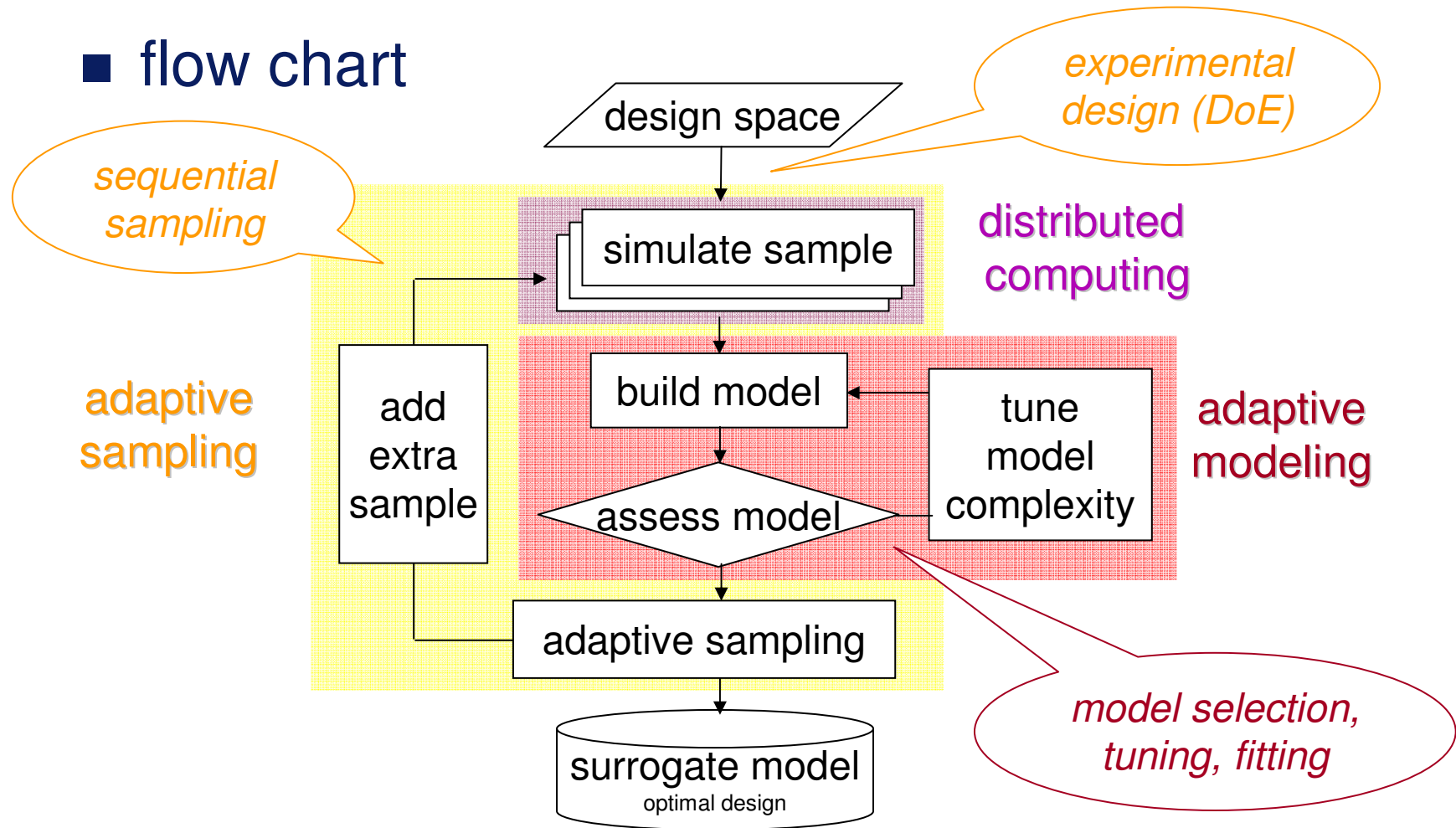
- traditional approach
 - classic optimization
 - ◆ not well suited for computational expensive simulations

■ Optimization

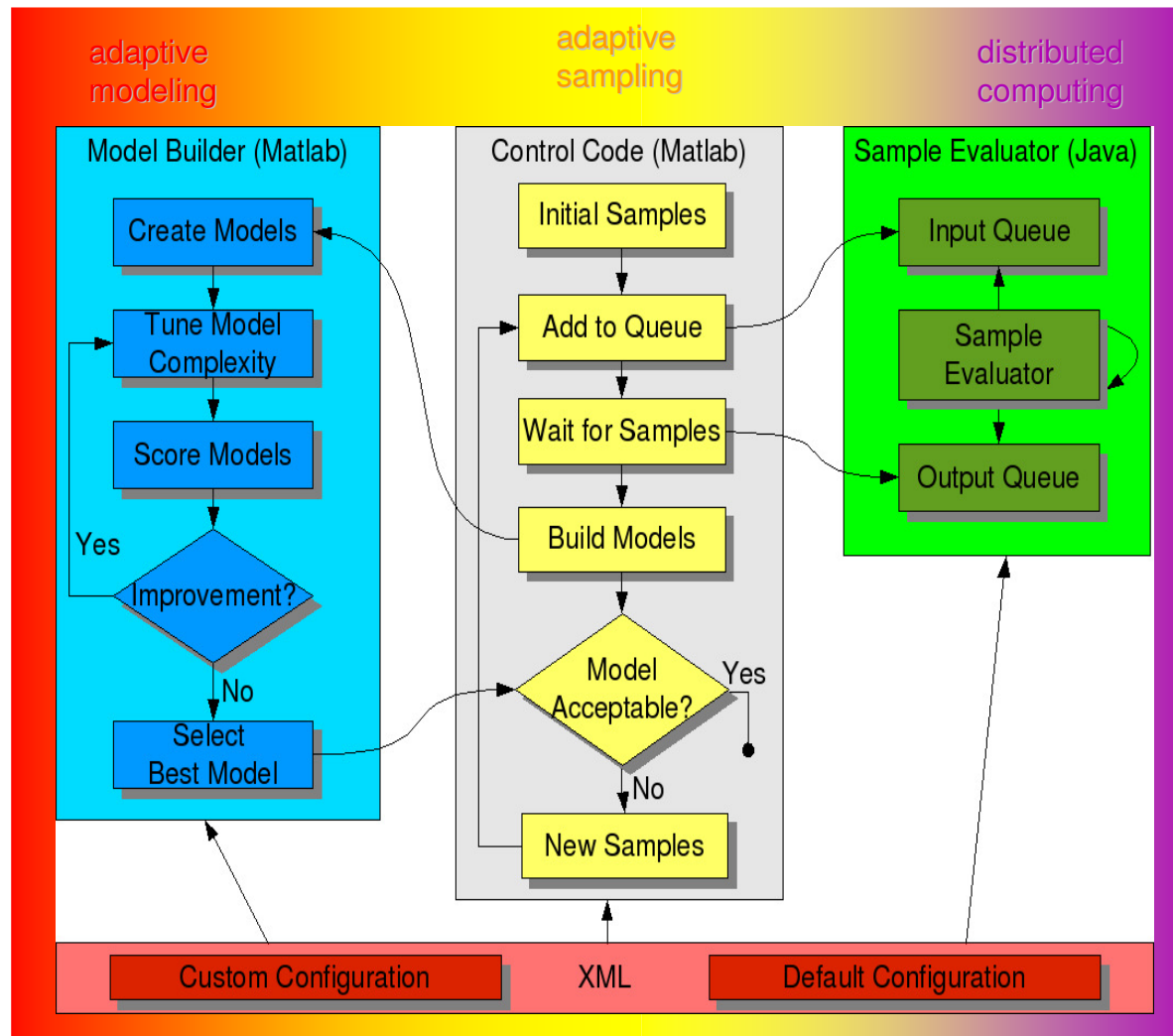
- surrogate-assisted optimization
 - ◆ global surrogate model
 - ◆ intermediate surrogate models & zoom-in



■ flow chart



- Who are we ?
- Introduction
- Surrogate modeling
- SUMO Toolbox
 - control flow & design
 - automatic model type selection
 - integrating gridcomputing
- Examples
- Conclusions



■ levels of pluggability

adaptive
modeling

- supports multiple model types
 - ◆ Polynomial/Rational functions
 - ◆ Artificial Neural Networks
 - ◆ RBF models
 - ◆ Support Vector Machines
 - ◆ (Blind) Kriging models
 - ◆ Splines
- modeling algorithm (NSGA-II, pattern search, GA, PSO, ...)
- model selection (crossvalidation, hold-out, R^2 , AIC, ...)

adaptive
sampling

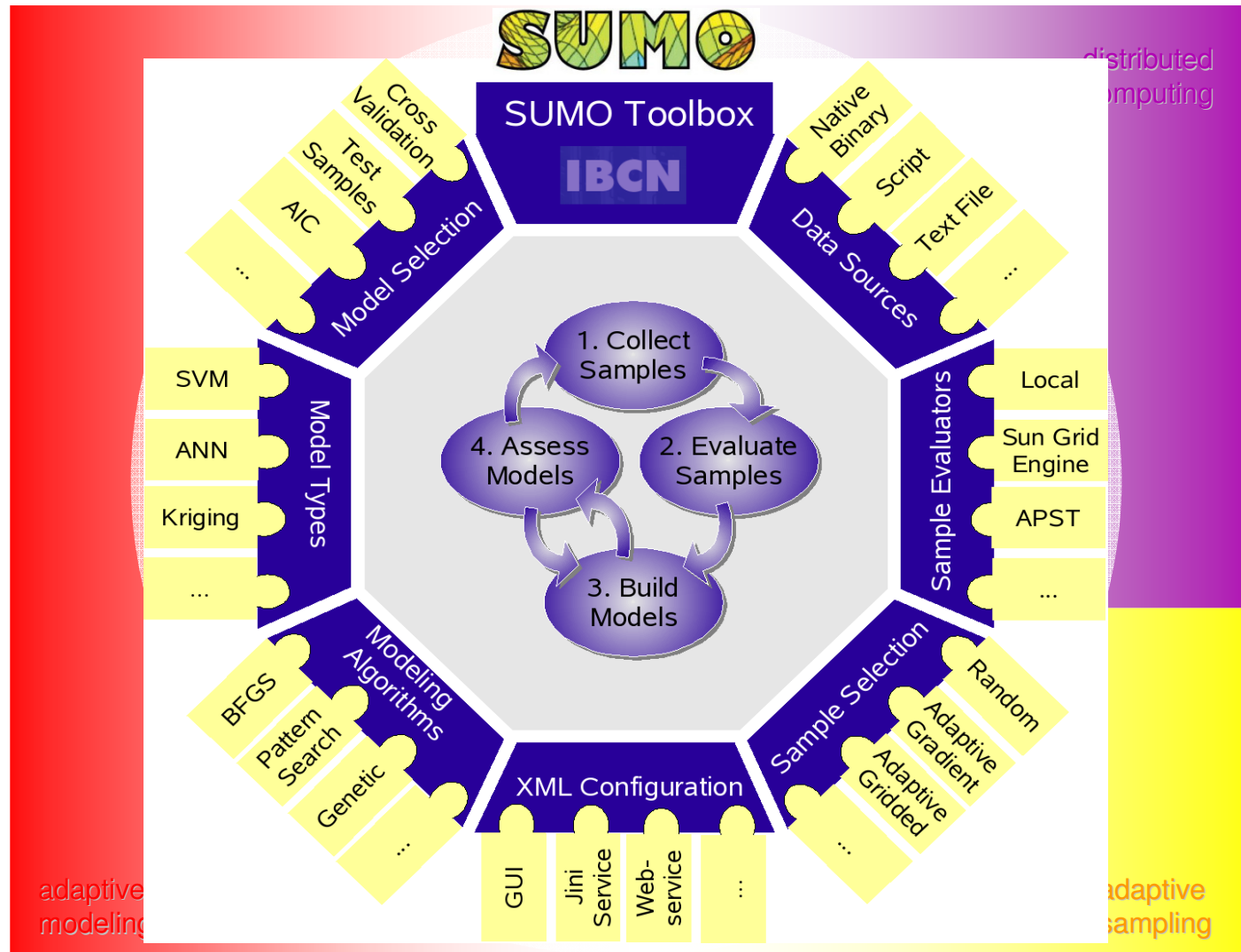
- initial experimental design (factorial, LHS, custom, ...)
- sequential design (error-based, density-based, hybrid, ...)

distributed
computing

- sample evaluation (local, distributed)

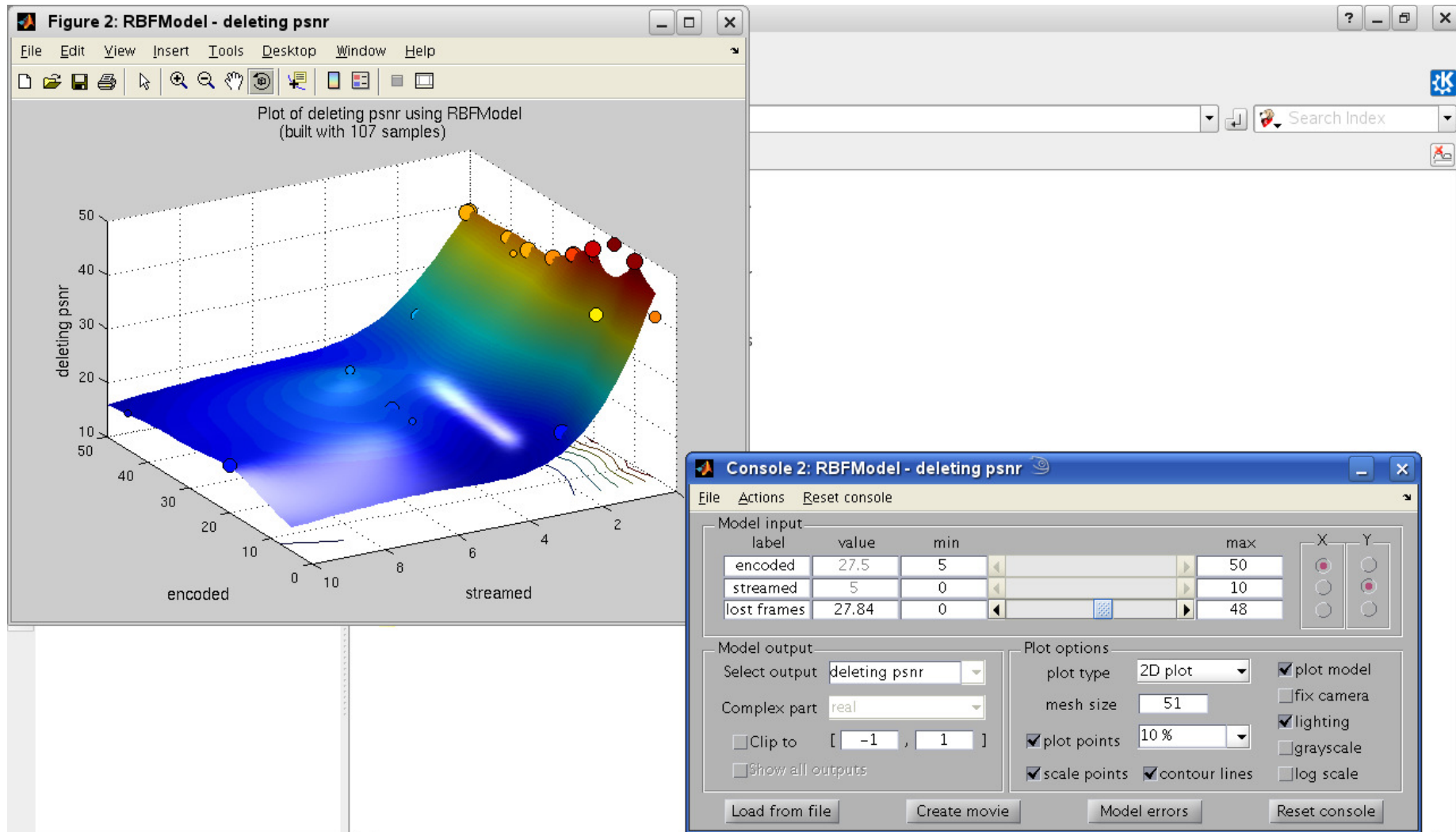
optimization

- multiple EGO criteria (GEI, EI, custom, ...)



■ SUMO Toolbox

- modular design to allow 3rd party extensions
 - ◆ **problem specificity can be controlled**
- powerful XML based configuration framework
 - ◆ **modeling primitives can be combined in many ways**
 - ◆ **sensible defaults but many 'expert' options available**
 - user remains in control
- extensive logging and profiling framework
 - ◆ **intermediate models (and plots) stored for further reference**
 - ◆ **understand behavior**
- GUI Tool for easy visualization and data exploration



■ however, which plugins to use?

- most important within adaptive modeling

■ many surrogate model types available:

- Rational functions, RBF models, Kriging, MLP, RBFNN, SVM, LS-SVM, regression trees, splines,

...

■ which type to use?

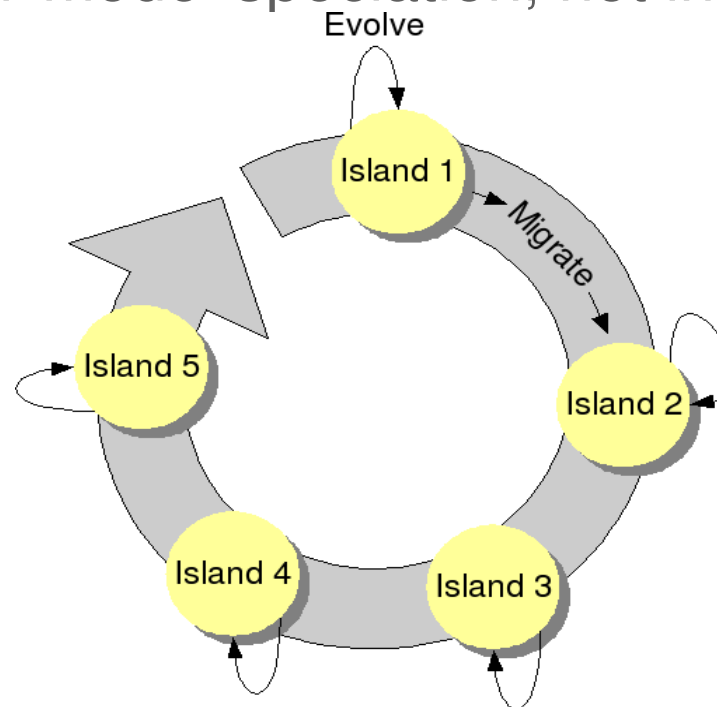
- problem & data dependent
- little theory available
 - ◆ e.g., rational functions and EM data
- usually pragmatic
- impossible to solve in general

- **each model is characterized by parameter set θ**
- **how to select θ_i ?**
 - by hand?
 - rule of thumb?
 - optimization algorithm?
 - ◆ BFGS, GA, pattern search, simulated annealing, PSO, ...
- **optimization landscape is dynamic!**
 - cfr. adaptive sampling

- **SUMO Toolbox makes it trivial to run and compare different methods**
- **however, an idea...**
 - Tackle the model type selection and model parameter optimization problem in one speciated evolutionary algorithm
- **let evolution decide**
 - survival of the fittest
 - multiple final solutions possible
 - hybrid solutions possible (cfr. ensembles)
- **interesting population dynamics?**

■ island model (migration model)

- most natural
- ring topology with different migration directions
- NB: inter-model speciation, not intra-model



■ heterogeneous recombination

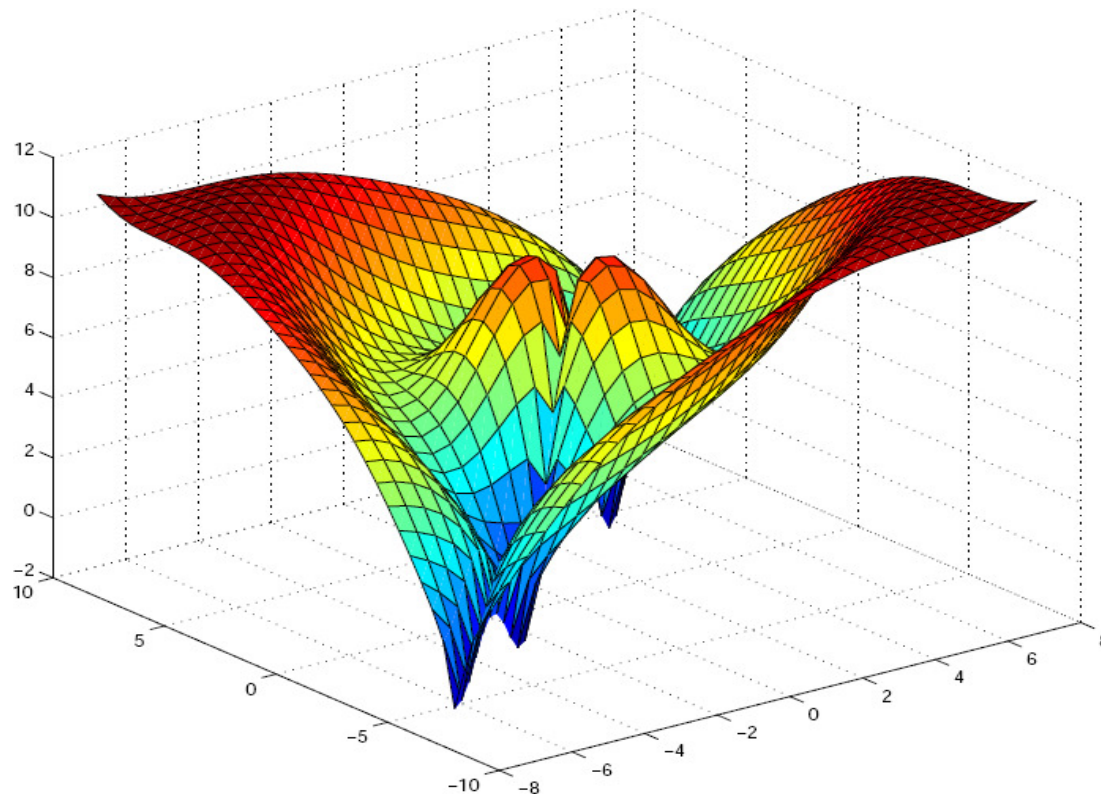
- Rational model x SVM = ???

■ use ensembles

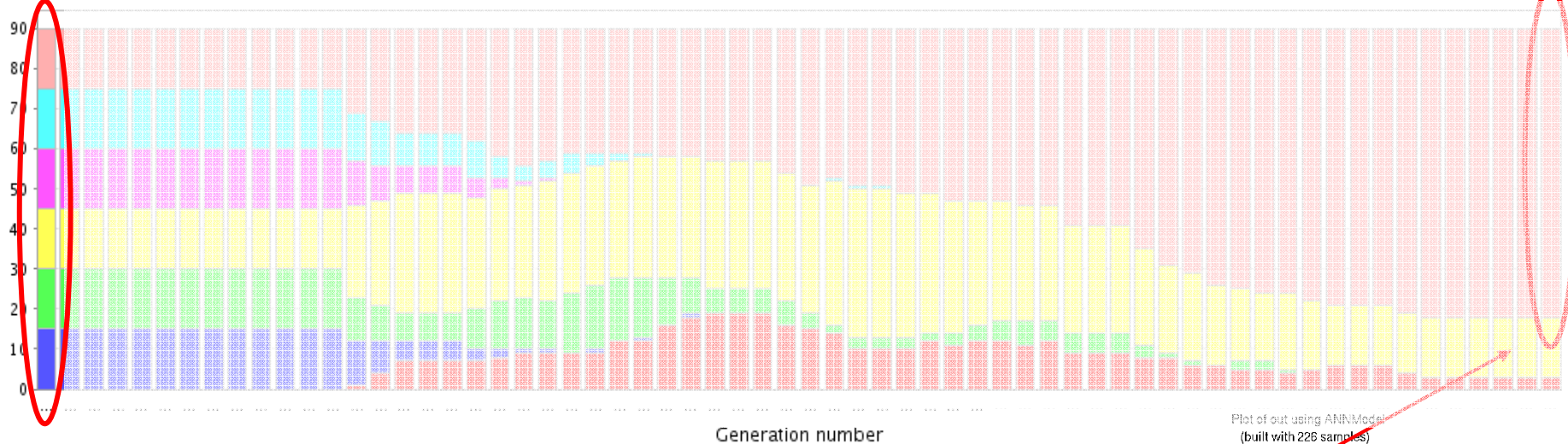
- phenotypic (behavioral) recombination
- avoid when possible
- many ensemble methods
 - ◆ **use simple average**
 - ◆ **others can easily be used instead**

■ 3D example ($z=0$)

$$f(x, y, z) = 7 \frac{\sin(\sqrt{x^2 + y^2}) + \epsilon}{\sqrt{x^2 + y^2}} + 3|x - y|^{1/2} + 0.01z$$



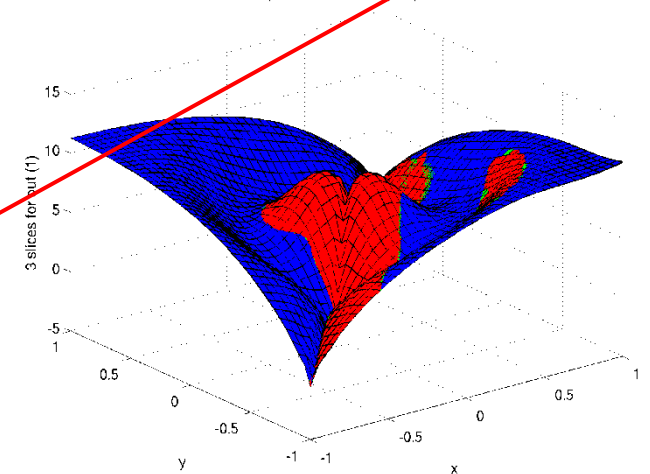
Profile for each generation



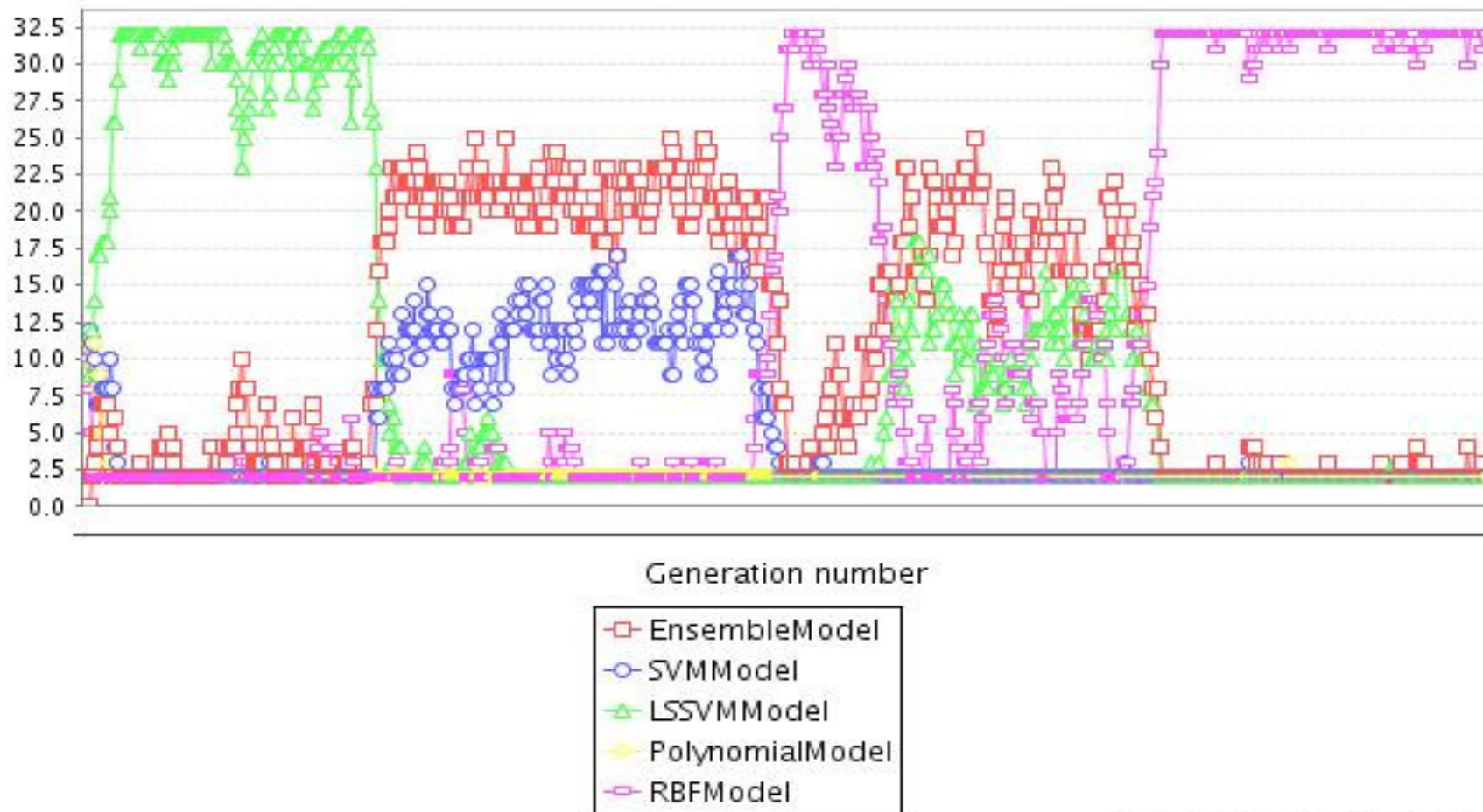
Model type selection

- start with 6 model types
- after multiple “generations”, favourable model(s) automatically selected

Plot of out using ANNModel
(built with 226 samples)



Profile for each generation



Generated using the M3-toolbox

- **promising results**
- **computation time \leq pure sequential**
- **delivers more insight**
- **however**
 - model type selection is not solved absolutely
 - ◆ **theoretically impossible without assumptions**
 - ◆ **GA meta parameters expected to be more robust**
 - sensitivity to migration/selection parameters?
 - constraints on reproducibility?

- **Ok, we have generated a model**
 - Why should you trust it?
- **Available assessment metrics depend on**
 - the model type
 - the problem requirements
- **In general if only data is available**
 - => data or response based generalization estimators (more than just accuracy!)
- **Some model types support more**
 - e.g., pole-zero rational models vs SVM
- **Golden standard : the domain expert**

- **The SUMO-Toolbox can support**
 - Whatever the model type supports
 - Any metric that can be expressed as a function
 - ◆ $metric(model) \rightarrow \mathbf{R}^n$
- **A metric can be..**
 - Checked manually at the end
 - Enforced during the model generation process
 - ◆ **As a constraint**
 - ◆ **As a penalty or score**
- **Note the ‘n’ in \mathbf{R}^n**
 - Multiple metrics can be combined
 - ◆ **Weighted sum**
 - ◆ **Multi-objectively**

- **stop once a good model is found**
- **problem: What is a good model?**
 - traditionally: one target accuracy/measure
 - e.g., average relative crossvalidation error of 5%
 - specified upfront

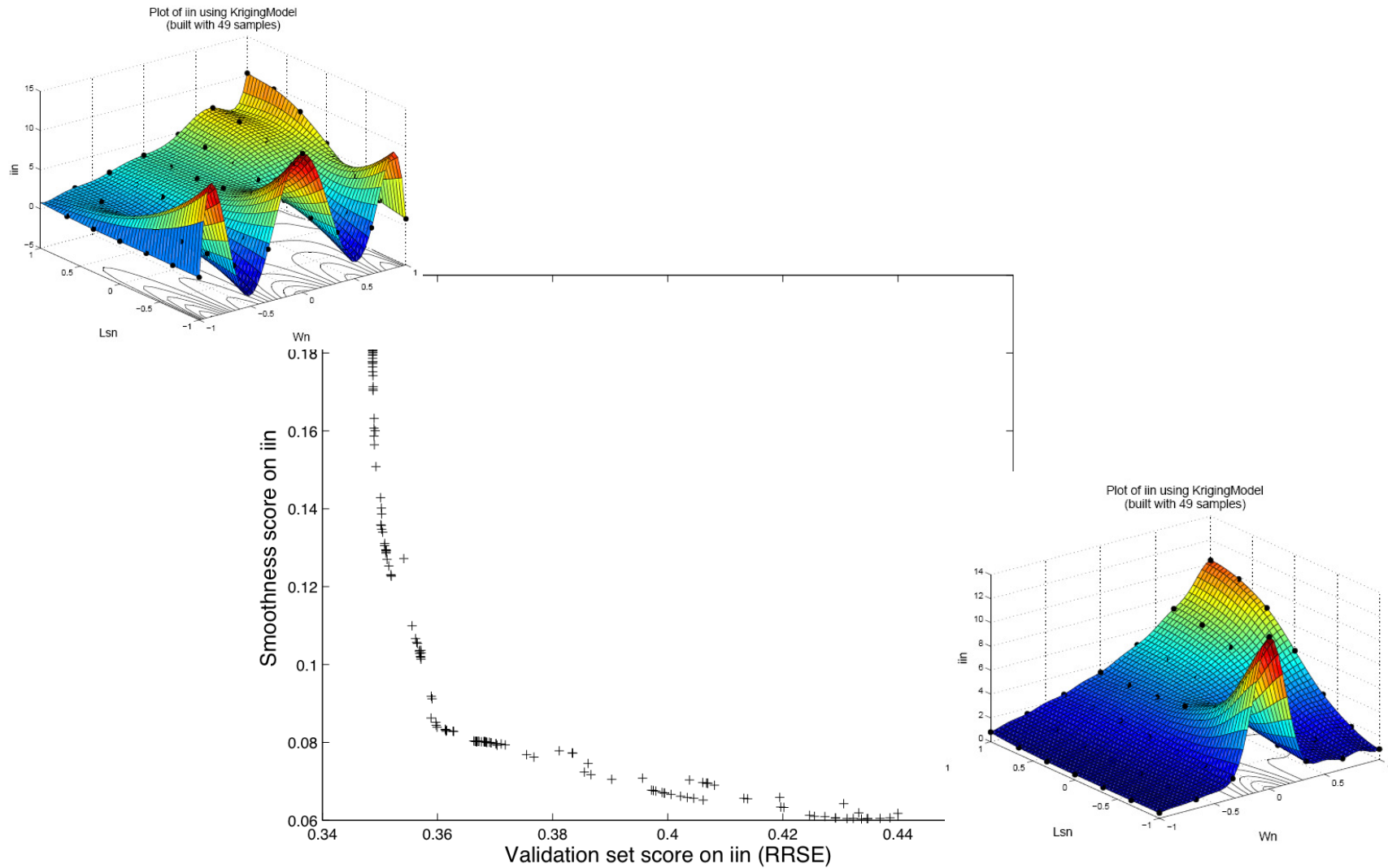


simplistic and impractical!

- many desirable model properties
 - ◆ **smoothness, accuracy, generalization, complexity, ...**
 - ◆ **may conflict**
- one metric cannot capture all requirements
- upfront specification is hard (interpretability)

■ **5% Problem**

- **model selection = inherently multi-objective**
- **different solutions**
 - scalarization, multi-level approach, multi-objective, hybrid, ...
 - each has different merits
- **multi-objective (MO) approach**
 - use standard MO algorithms for hyperparameter optimization (NSGA-II, AMALGAM, ...)
 - multi-output modeling
 - ◆ enables automatic model type selection per output
- **extension: dynamic number of objectives**



■ Simulations are expensive

- Adaptive sampling
- 1-time up front investment
- Provide interface to the grid

■ Goal

- Transparent integration
- Avoid middleware lock-in
- Hide grid details

■ Integration on 3 levels

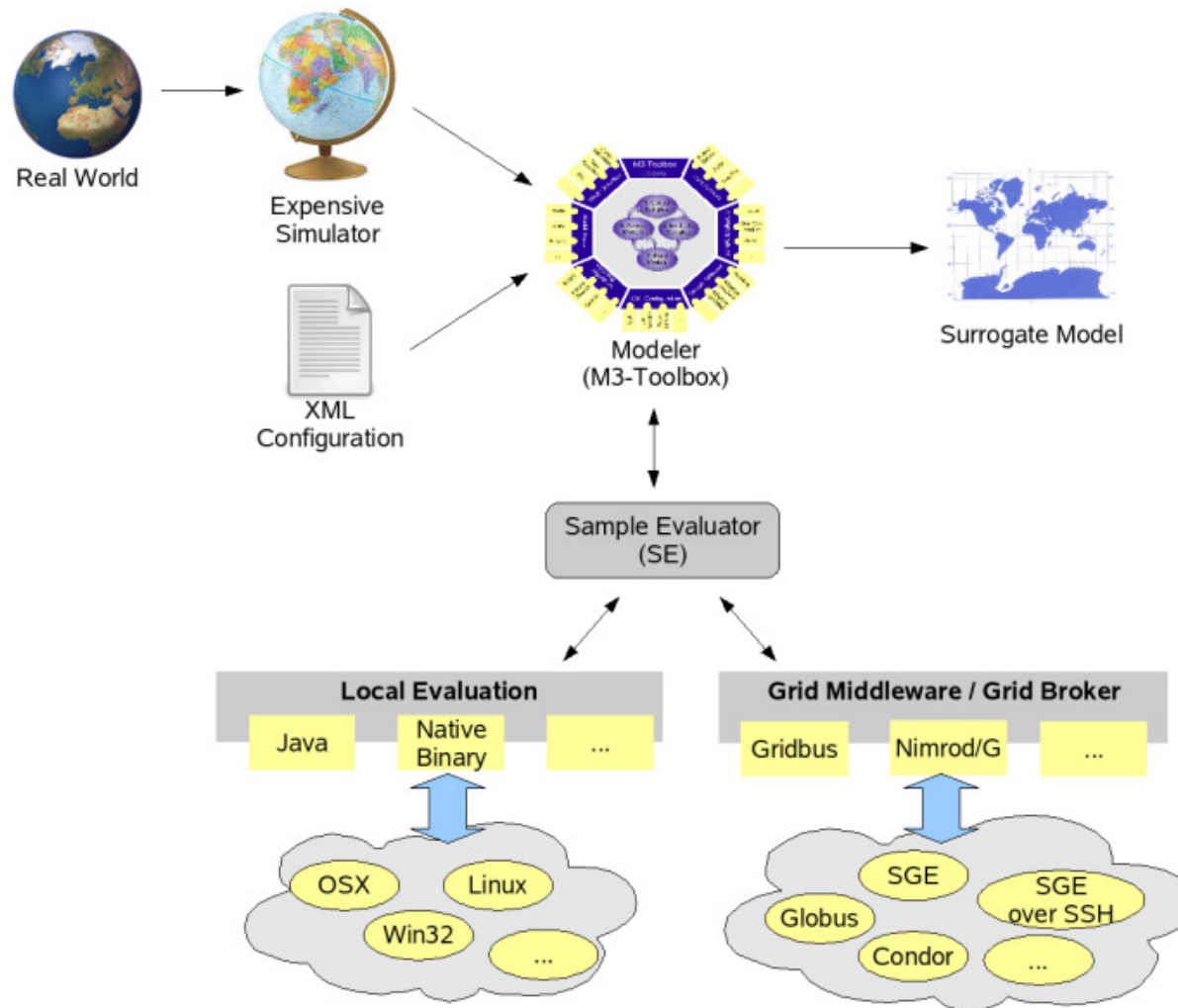
- Resource level
- Scheduling level
- Service level

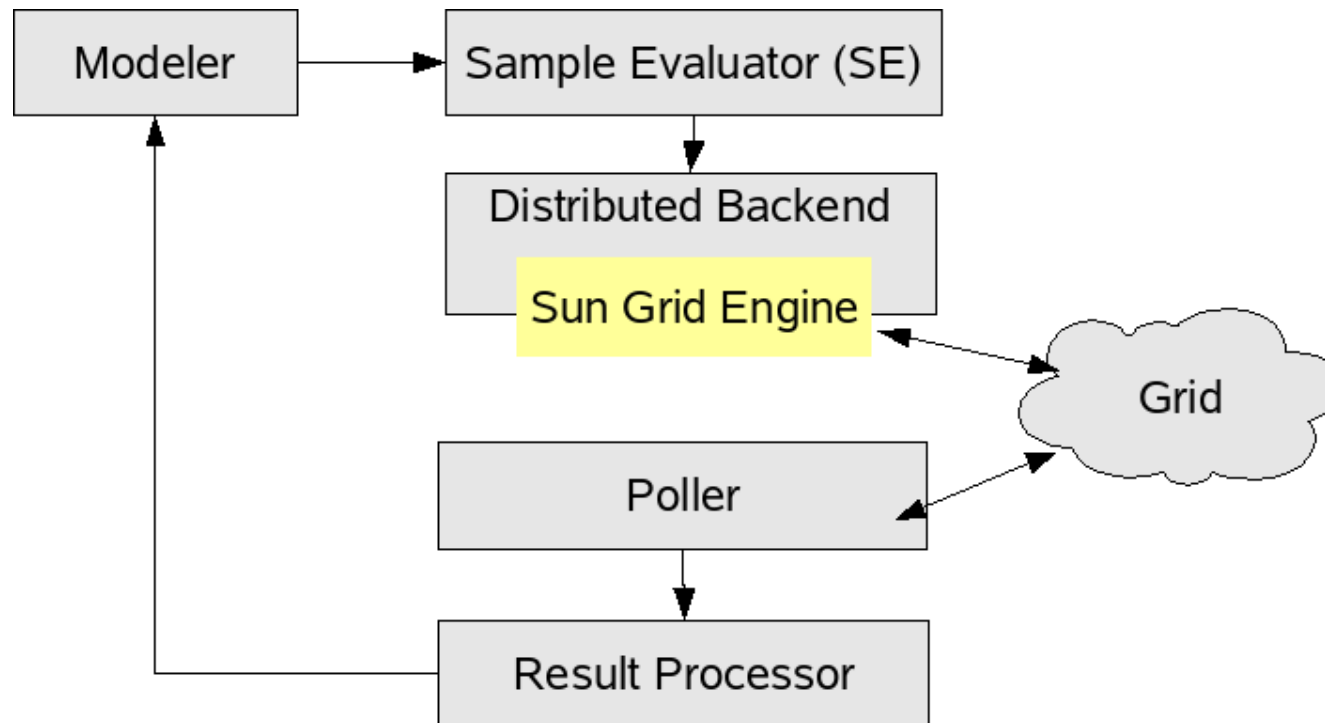
■ resource level

- raw distribution
- un simulations in parallel

■ SampleEvaluator abstraction

- cfr. flow chart
- clean object oriented interface
- translates modeler requests into middleware specific jobs
- support multiple backends
 - ◆ Sun Grid Engine
 - ◆ LCG middleware
 - ◆ APST





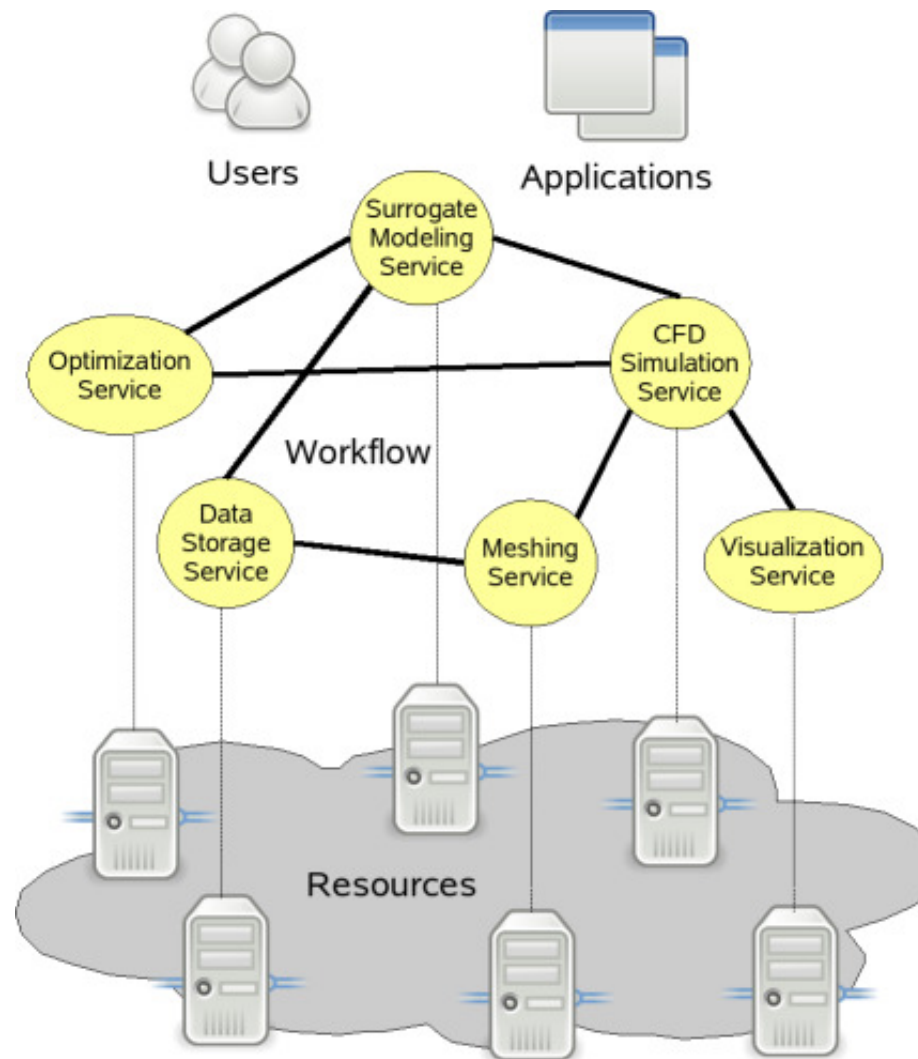
■ scheduling level

- data points have different priorities
 - ♦ e.g., domain borders, optima, sparse regions, ...
- compute resources are heterogeneous
- resources are shared (dynamic!)
- integrate grid resource information and modeling information into scheduling decisions

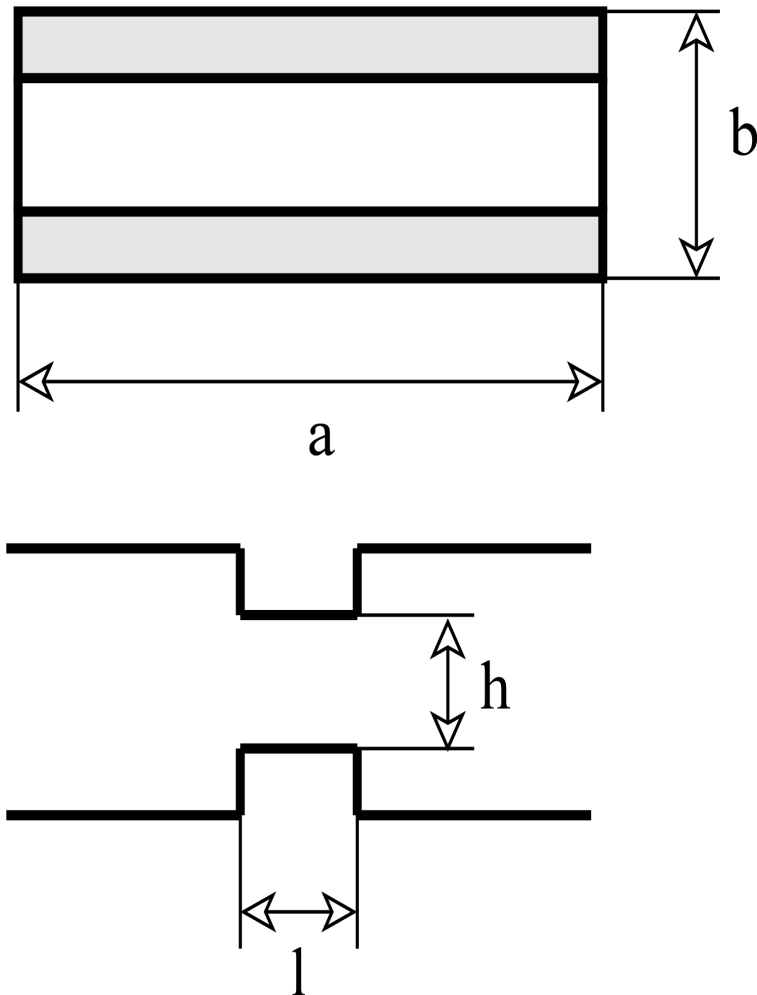
➡ Application and resource aware scheduling

■ service level

- integration as part of a larger service oriented architecture (SOA)
- easy access and integration into the design process
 - ◆ **web browser, Jini, SOAP, ...**
- complicated workflows possible



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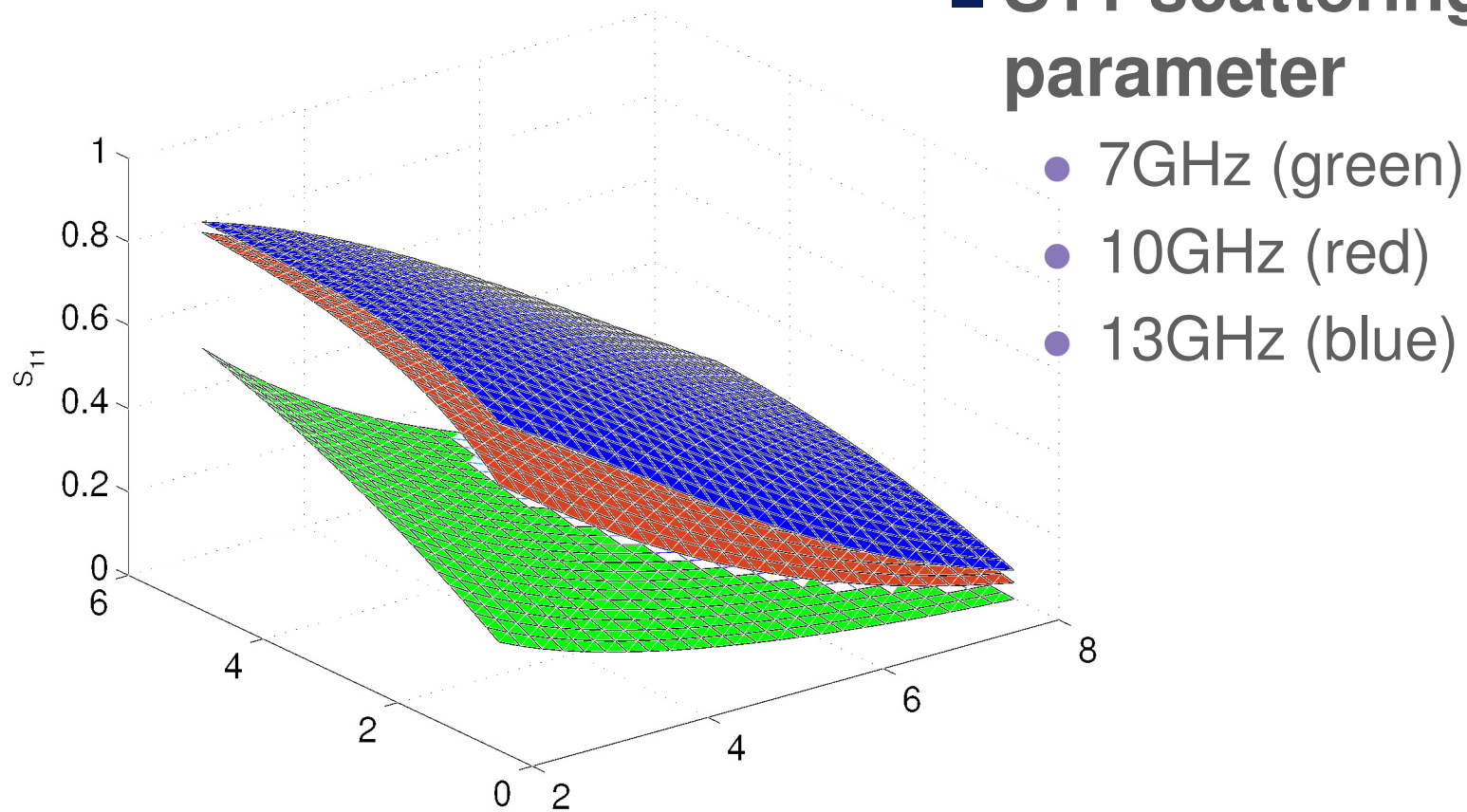
■ Step discontinuity in a rectangular waveguide

- Frequency : 7-13 GHz
- Step length [l] : 2-8 mm
- Gap height [h] : 0.5-5 mm
- Waveguide width [a] : 22.86 mm
- Waveguide height [b] : 10.16 mm

■ Distributed backend:

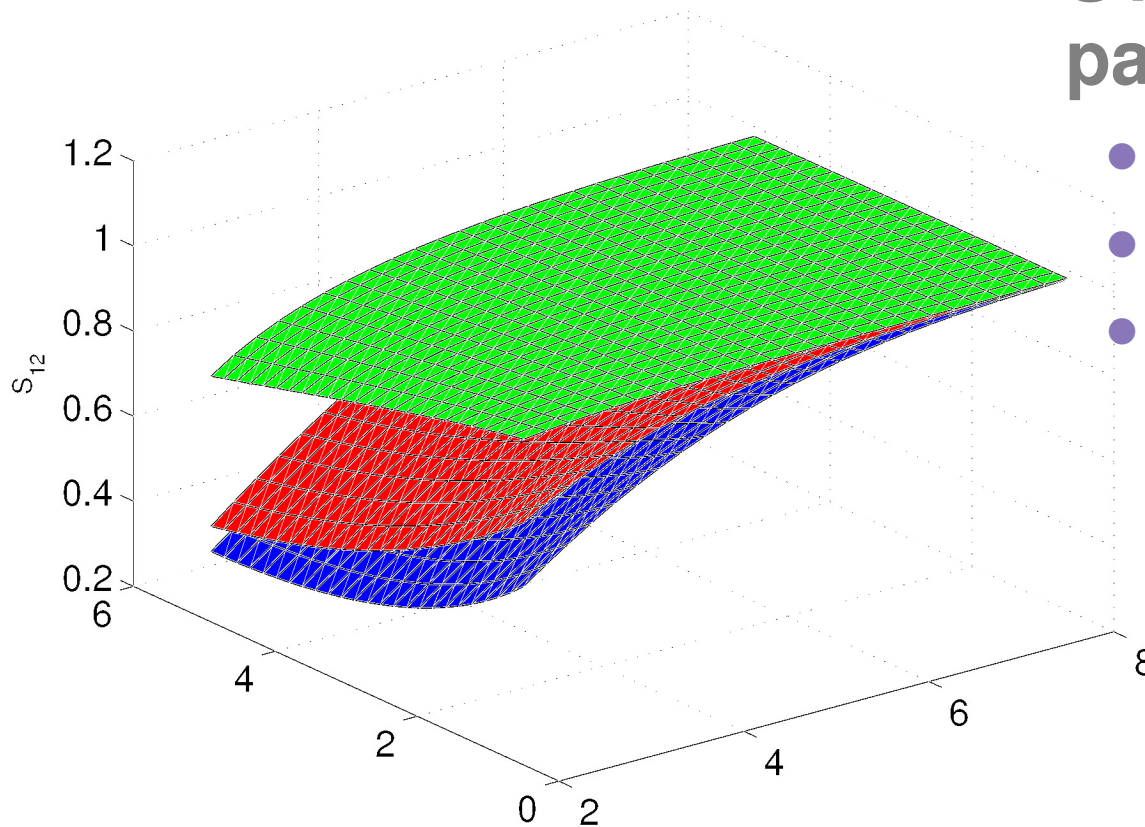
- Remote 256 node SGE cluster

■ S11 scattering parameter



■ S12 scattering parameter

- 7GHz (green)
- 10GHz (red)
- 13GHz (blue)



<Simulator>

<Name>Step Discontinuity</Name>

<InputParameters>

<Parameter name="frequency" type="real" minimum="7" maximum="13"/>

<Parameter name="gapHeight" type="real"/>

<Parameter name="stepLength" type="real"/>

</InputParameters>

<OutputParameters>

<Parameter name="S11" type="complex"/>

<Parameter name="S12" type="complex"/>

</OutputParameters>

<Implementation>

<Executable platform="unix" arch="amd64">StepDiscontinuity</Executable>

<DataFiles>...</DataFiles>

</Implementation>

</Simulator>

```
<ToolboxConfiguration version="6.1">
```

```
  <Plan>
```

```
    ...
```

```
    <SampleSelector>gradient</SampleSelector>
```

```
    <Measure type="CrossValidation" target=".0001" errorFcn="absoluteRMS" use="on" />
```

```
    ...
```

```
  <Run>
```

```
    <Simulator>StepDiscontinuity.xml</Simulator>
```

```
    <SampleEvaluator>sge</SampleEvaluator>
```

```
  <Outputs>
```

```
    <Output name="S11" complexHandling="complex">
```

```
      <AdaptiveModelBuilder>poly</AdaptiveModelBuilder>
```

```
    </Output>
```

```
    <Output name="S12" complexHandling="split">
```

```
      <AdaptiveModelBuilder>kriging</AdaptiveModelBuilder>
```

```
    </Output>
```

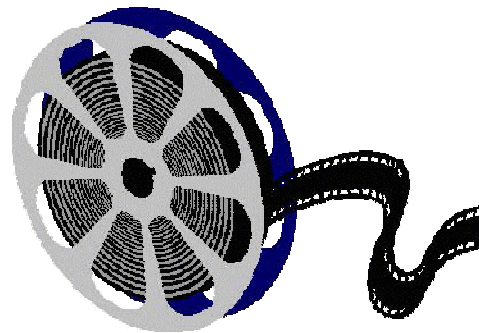
```
    <Output name="S11,S12" complexHandling="modulus">
```

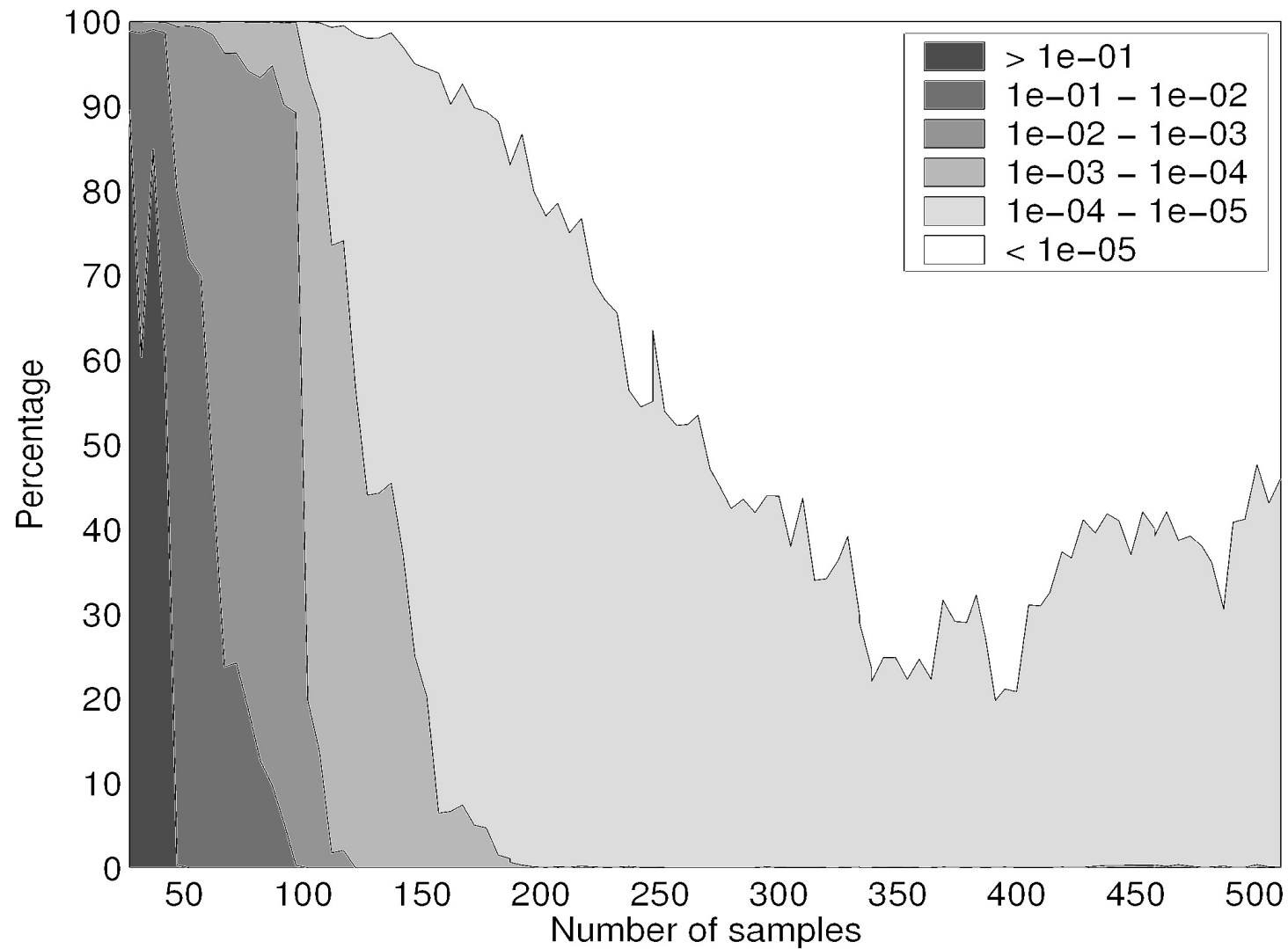
```
      <AdaptiveModelBuilder>anngenetic</AdaptiveModelBuilder>
```

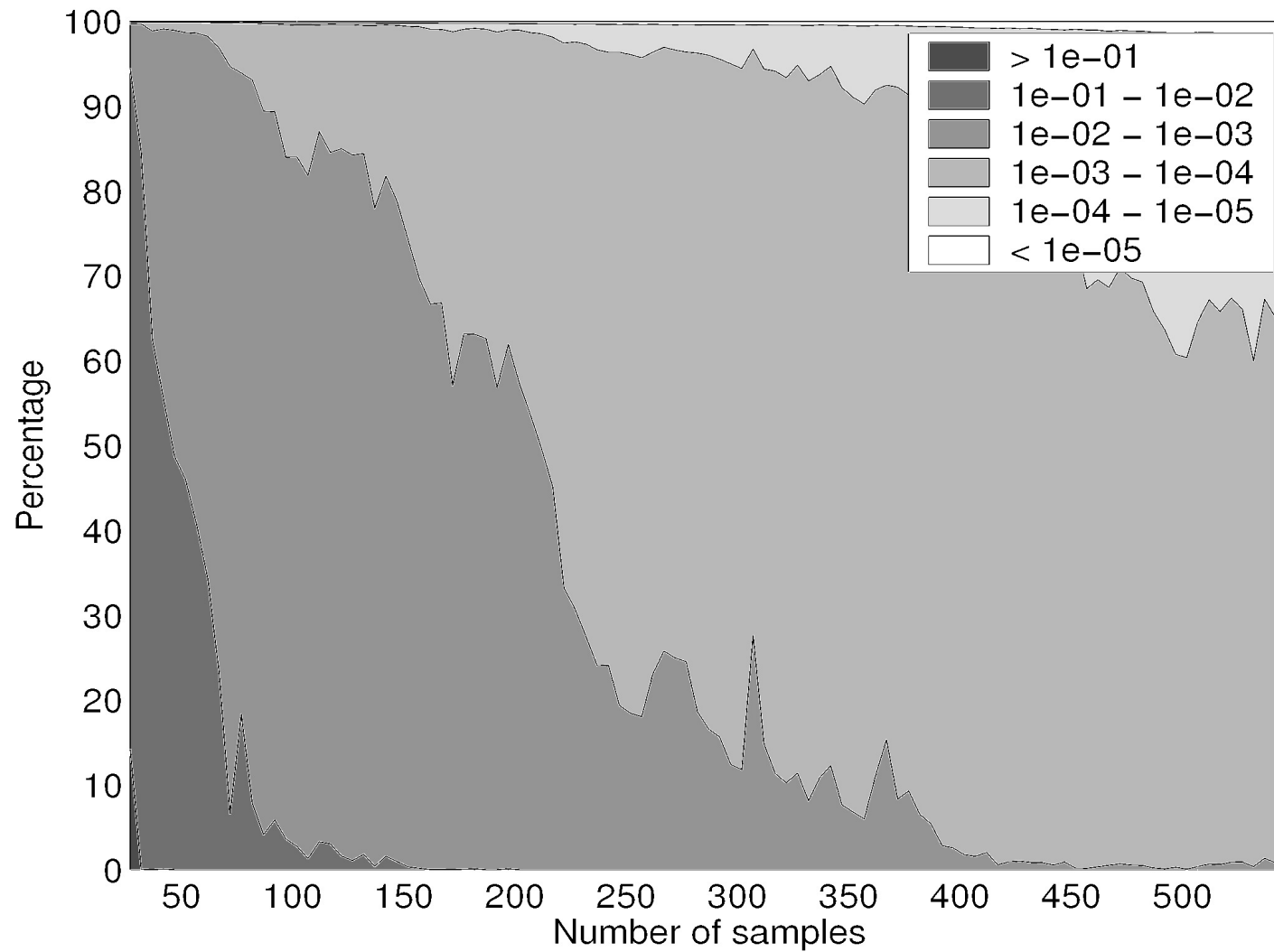
```
    </Output>
```

```
  </Outputs>
```

```
  ...
```

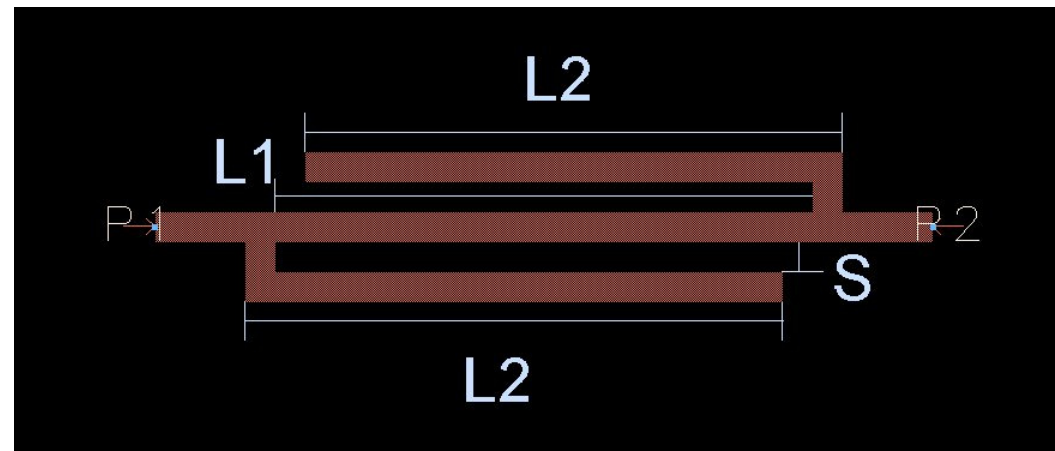







■ Double-folded microstrip stub bandstop filter (see Bandler 1994)

- Model scattering parameters
- Simulated with ADS Momentum
 - ♦ Input: L1, L2, frequency
 - ♦ Output: S11, S12

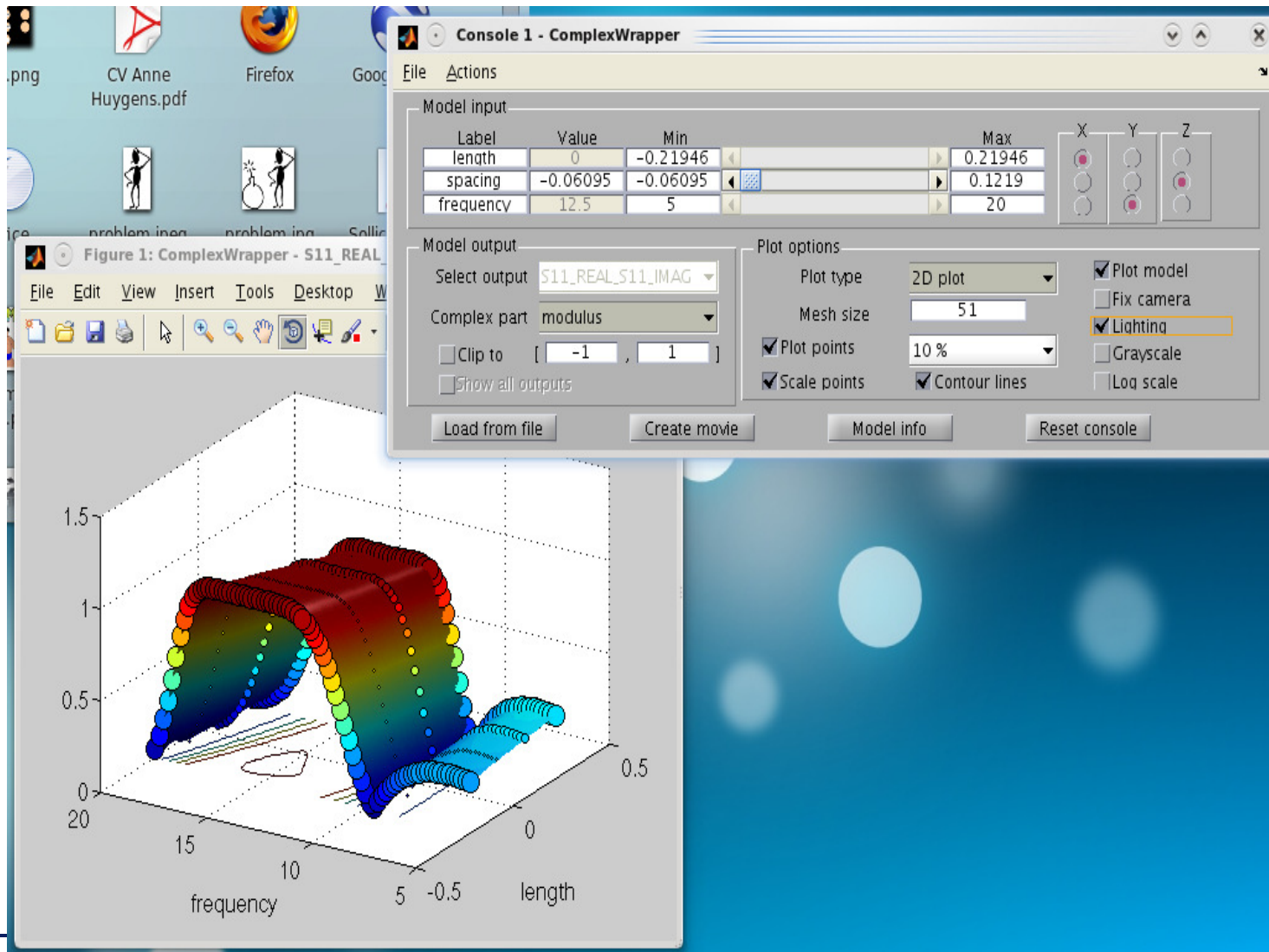


■ Experimental setup

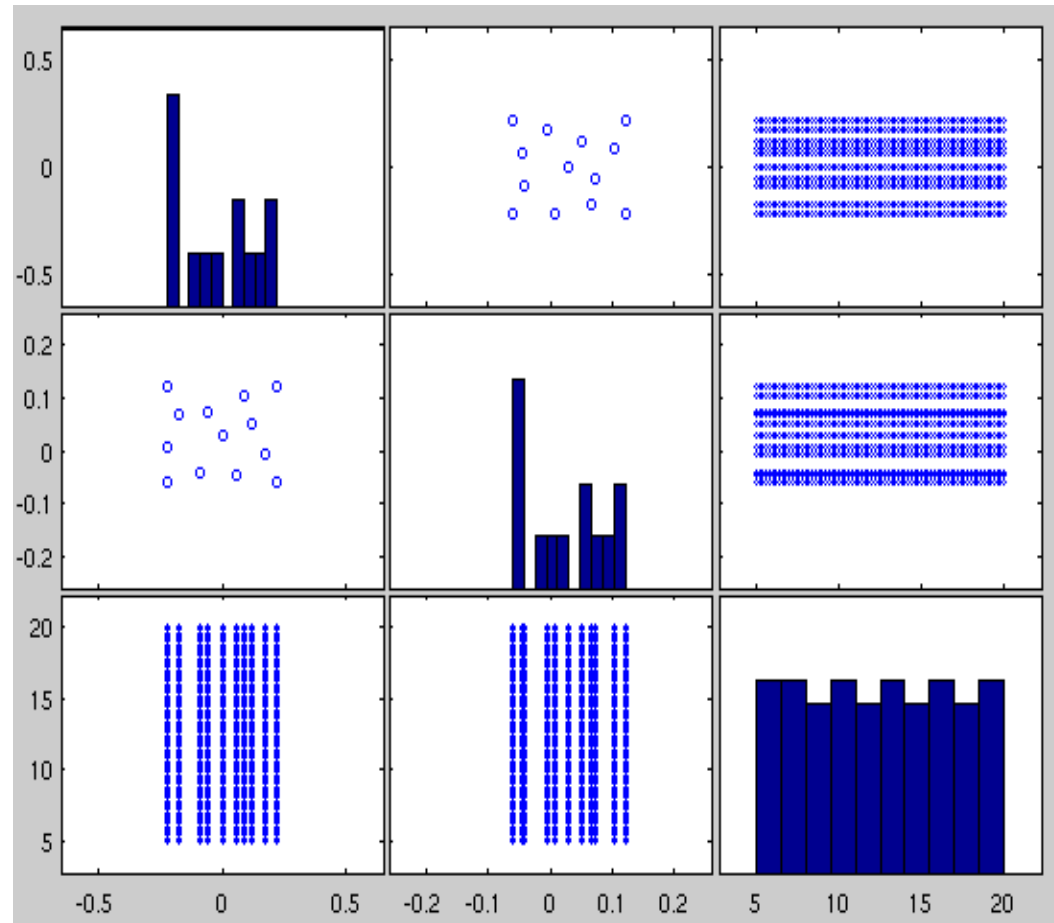
- Model with ANN
 - ◆ topology selected automatically using a GA
 - ◆ Minimize (LRM + in-sample error)
- Select samples using a combination of
 - ◆ **Error based sampling and gradient based sampling**
 - Select samples where the model is uncertain and the response is non-linear

■ Important

- Momentum = a frequency domain solver
 - ◆ Frequency is sampled automatically
- => only sample in L1-L2 space



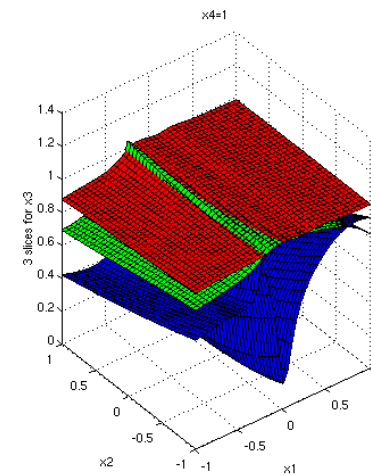
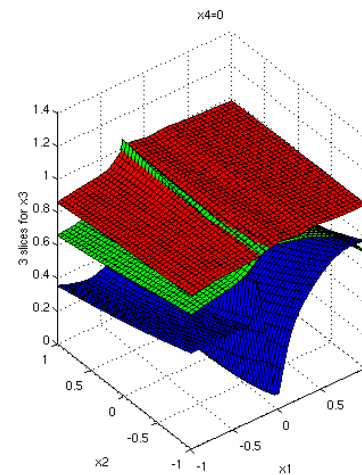
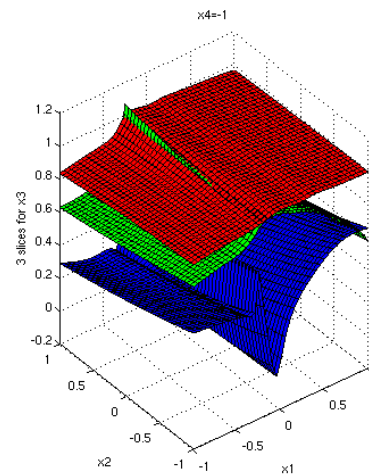
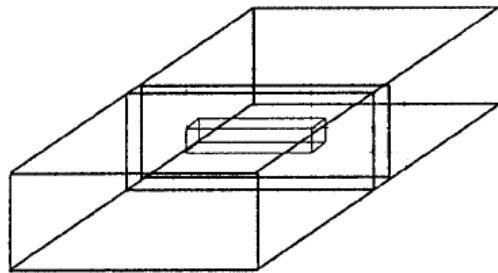
■ Sample distribution



■ iris in rectangular waveguide (From Lamecki 2005)

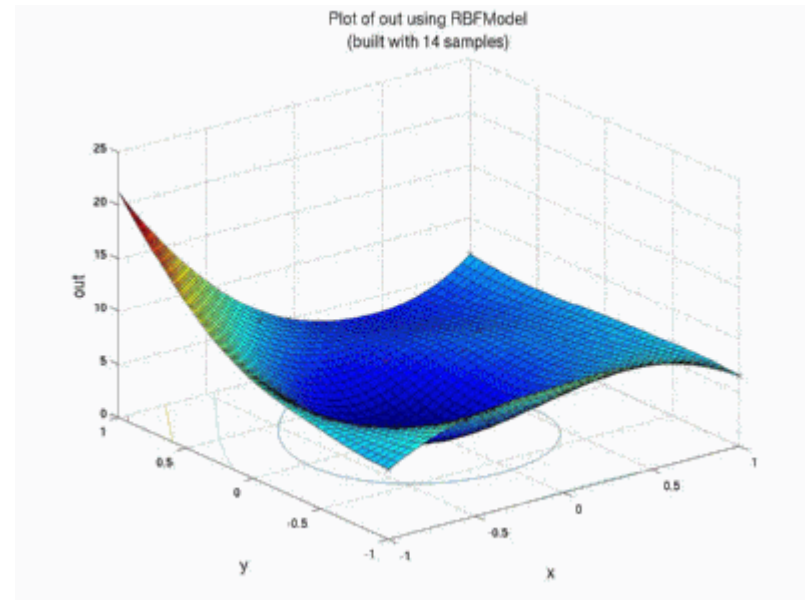
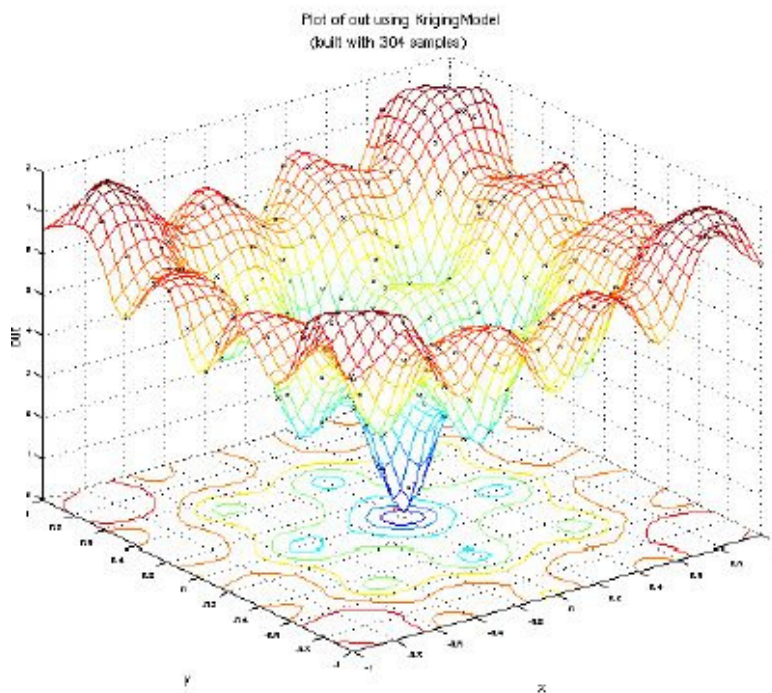
● Simulation of scattering parameters

- ◆ Input : frequency, iris height, length, width,
- ◆ Output : S11, S12



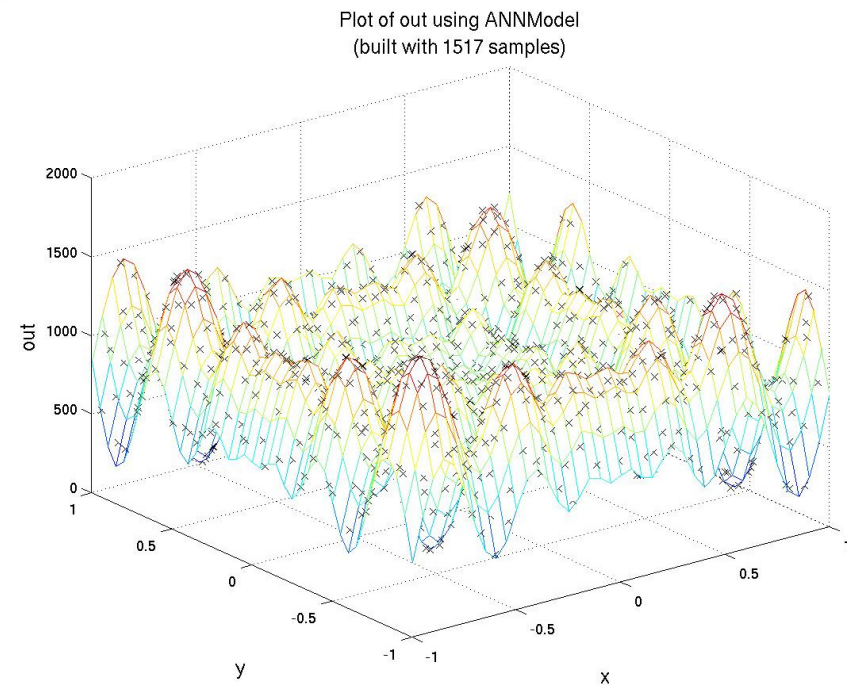
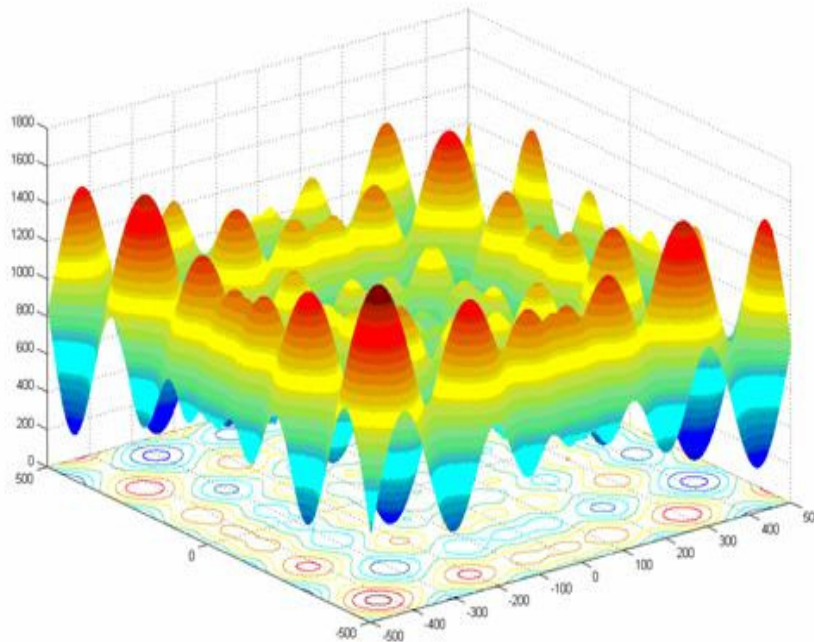
■ Ackley function

- Classic 2D test function from optimization



■ Schwefel Function

- Classic 2D test function from optimization



■ methane – air combustion (From Ihme 2007)

● Simulation of temperature

- ◆ Input : mixture fraction variable z ,
reaction progress variable c
- ◆ Output : temperature

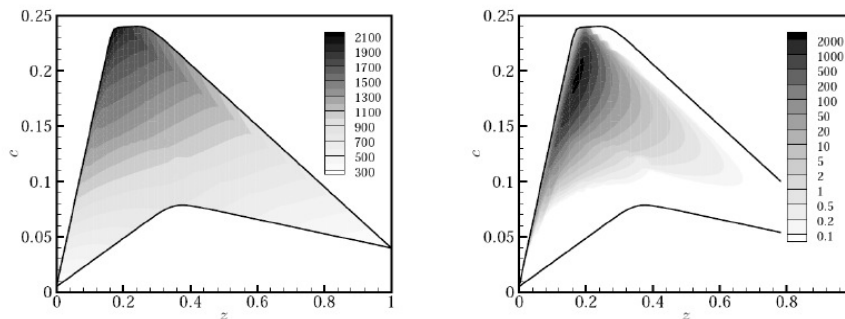
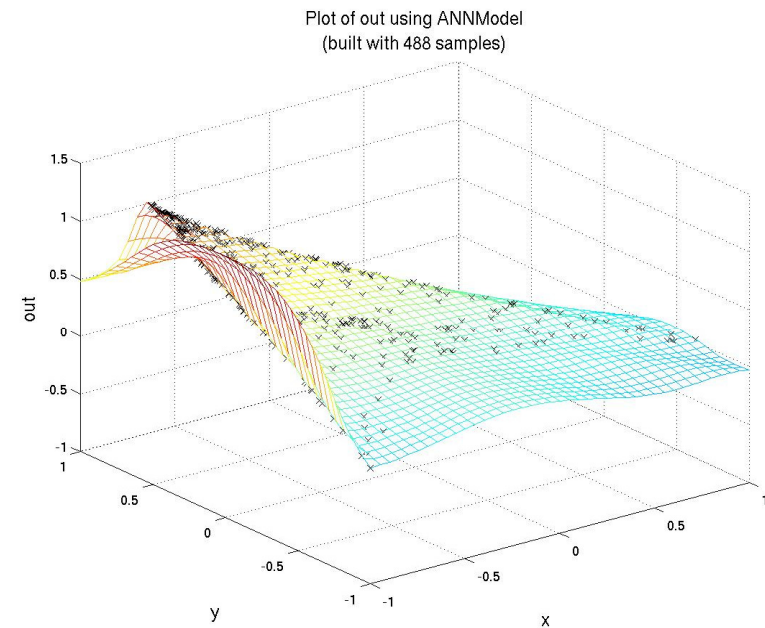


Figure 5.3: Solution of the steady laminar flamelet equations as a function of mixture fraction z and progress variable c ; (a) temperature (K) and (b) chemical source term ($kg/(m^3s)$) (Source: [77])



■ re-usable Langly Glide Back Booster (LGBB)

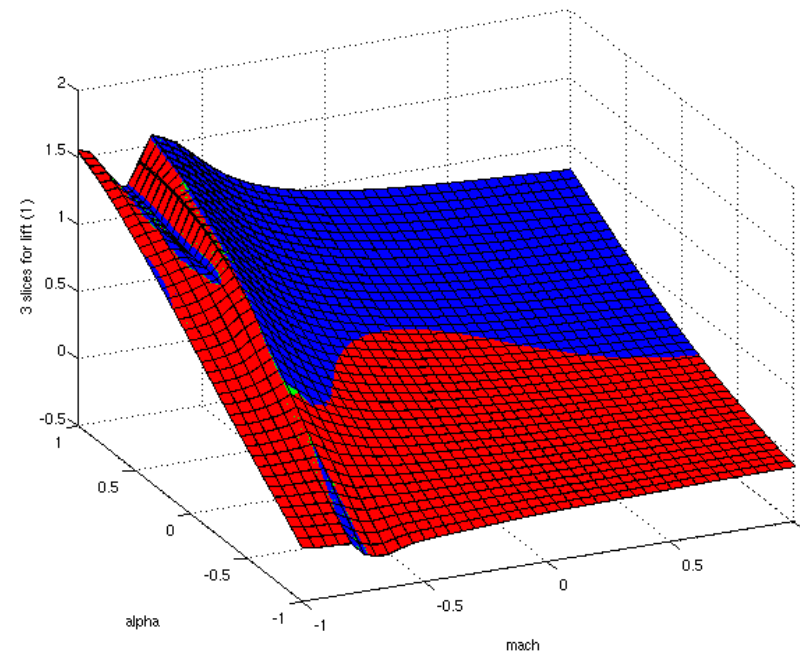
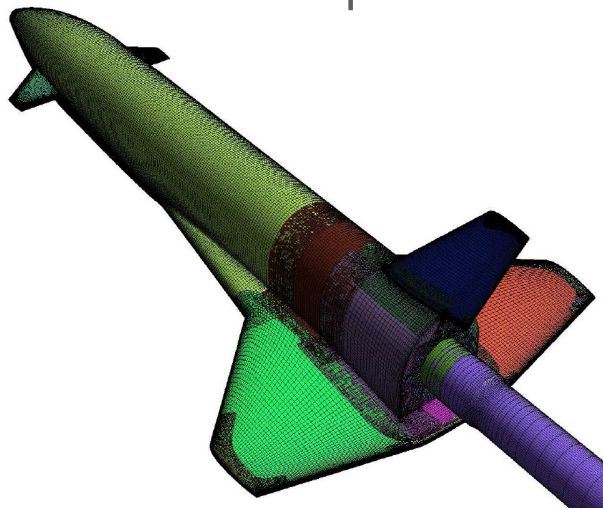
(From Gramancy 2004 / NASA)

● Simulation of lift

- ◆ Input
angle
- ◆ Output : lift

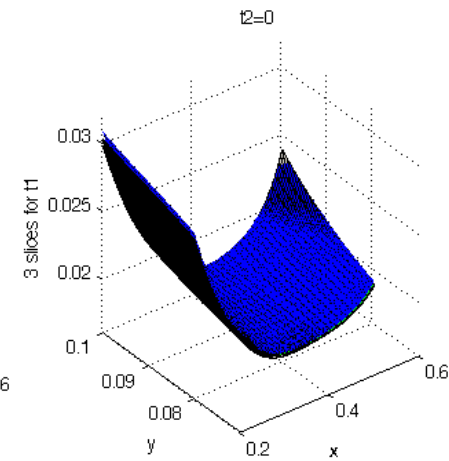
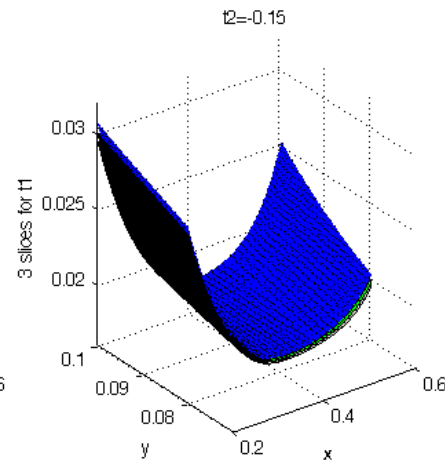
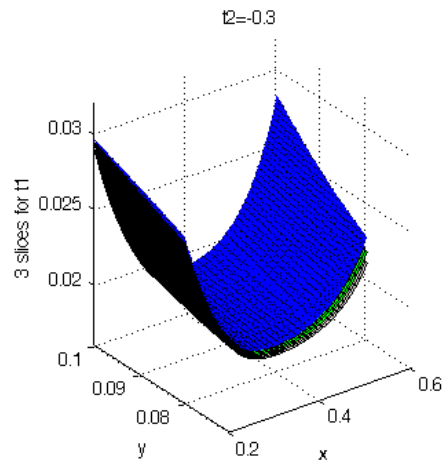
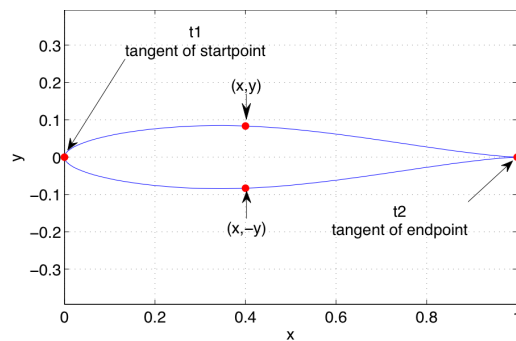
: mach number, angle of attack, slip slide

Plot of lift using ANNModel
(built with 780 samples)

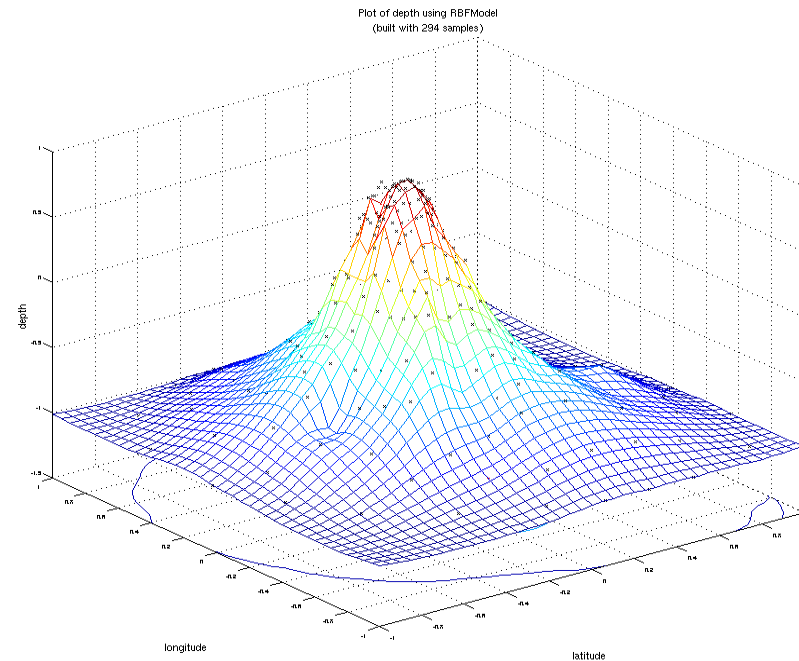


■ Xfoil – subsonic airfoil development (Xfoil)

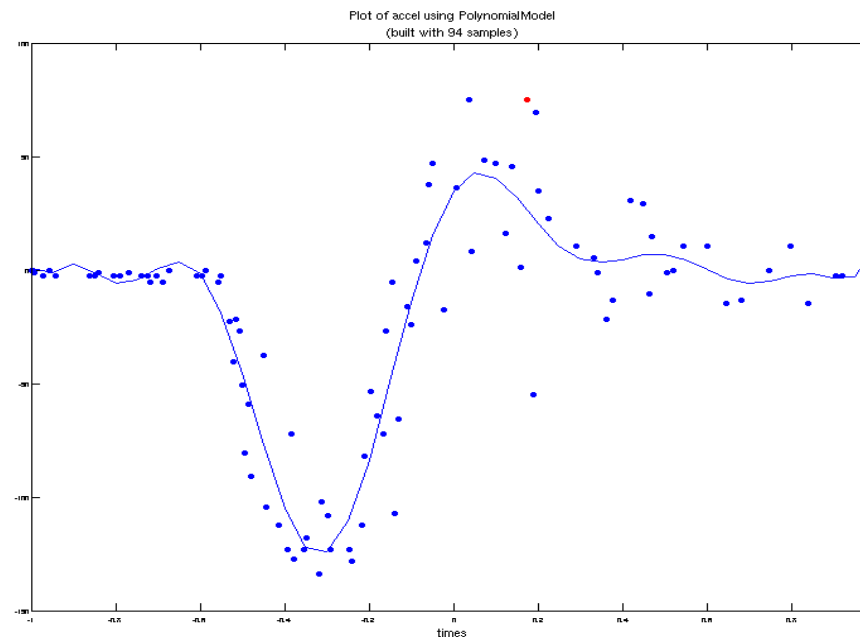
● Model drag on Wheel-Fairing airfoil



- **seamount** (From Parker 1987)
 - Elevation data from a submerged mountain
 - ◆ Input : latitude, longitude
 - ◆ Output : depth



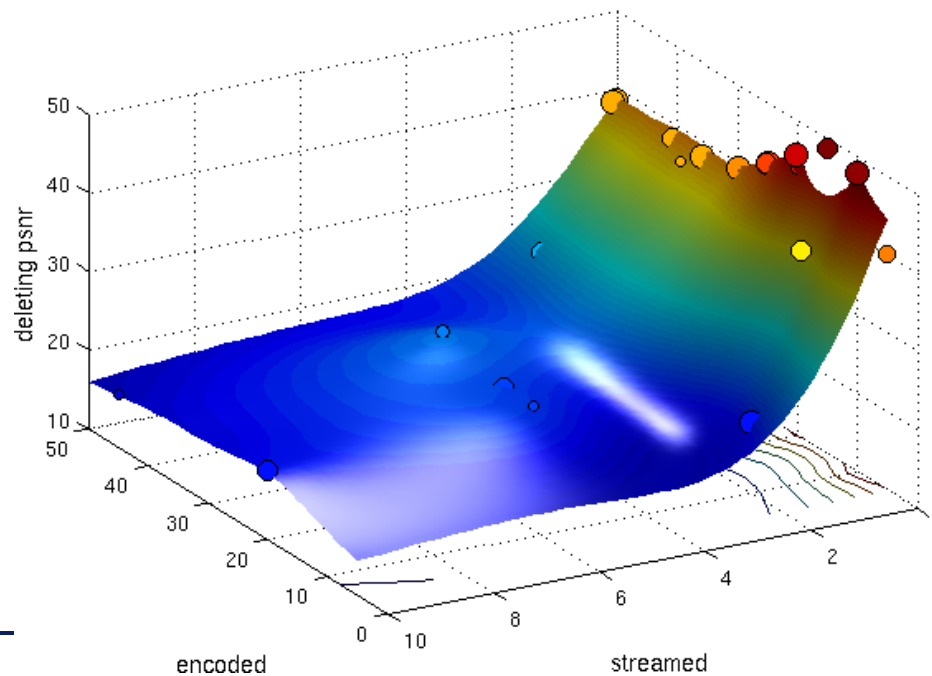
- **motorcycle accident** (From Silverman 1987)
 - Simulate a motorcycle crash against a wall
 - ◆ Input : time in milliseconds since impact.
 - ◆ Output : the recorded head acceleration (in g)



■ Video quality data (From Nick Vercammen, IBBT)

- How does streaming/encoding affect quality
 - ◆ Input : encoding, transmission parameters
 - ◆ Output : quality metric

Plot of deleting psnr using RBFModel
(built with 107 samples)

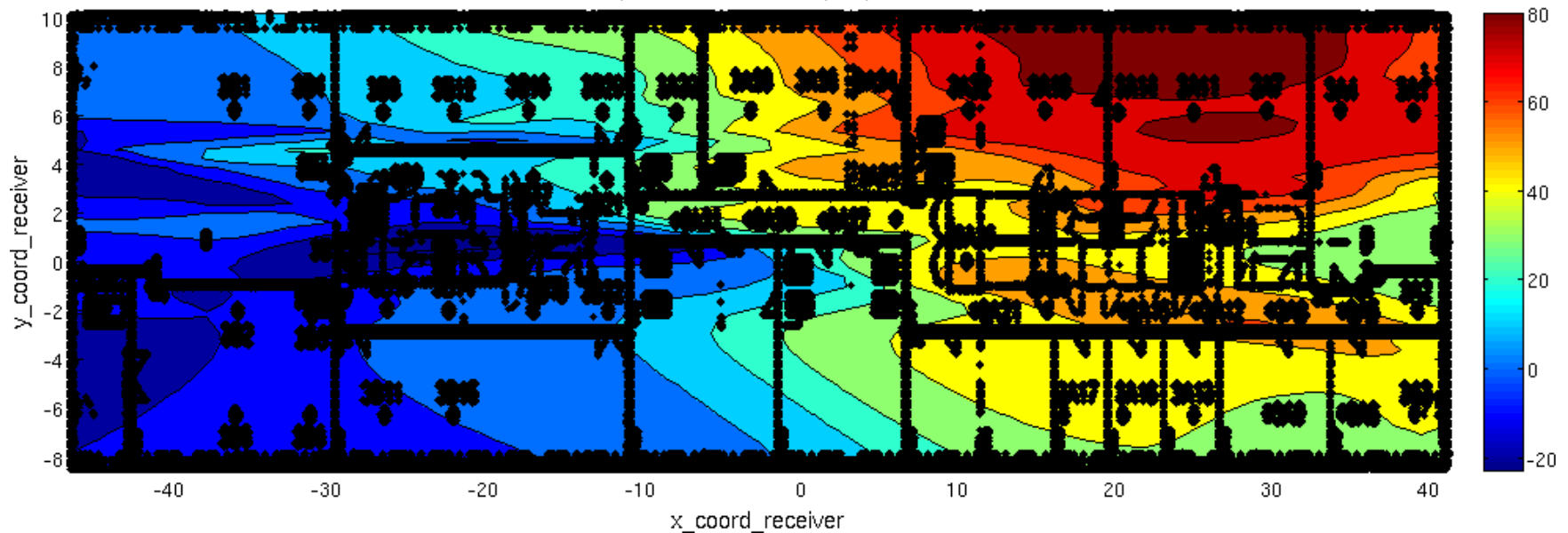


■ Wireless sensor data (From Sensor Lab, IBBT)

- Model reception quality

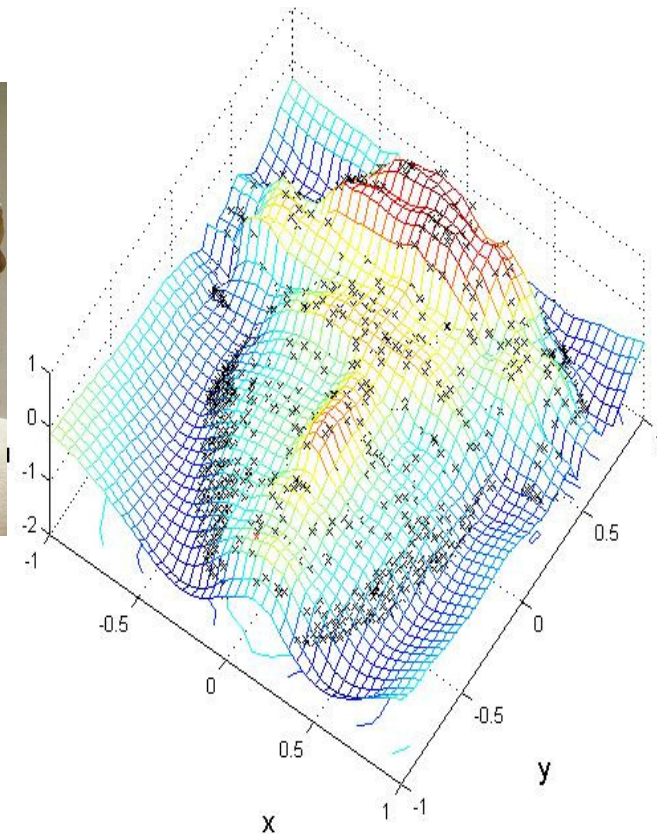
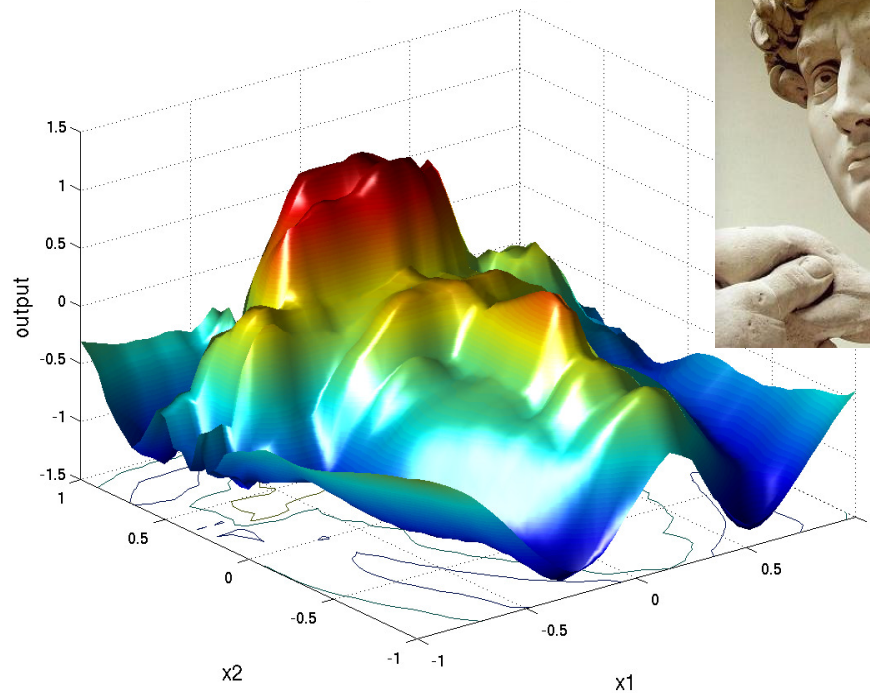
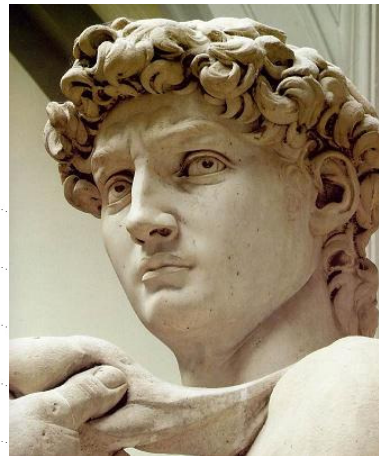
- ◆ Input : sender/receiver coordinates
- ◆ Output : reception quality metric

Plot of avg_LQI using ANNModel
(built with 29646 samples)



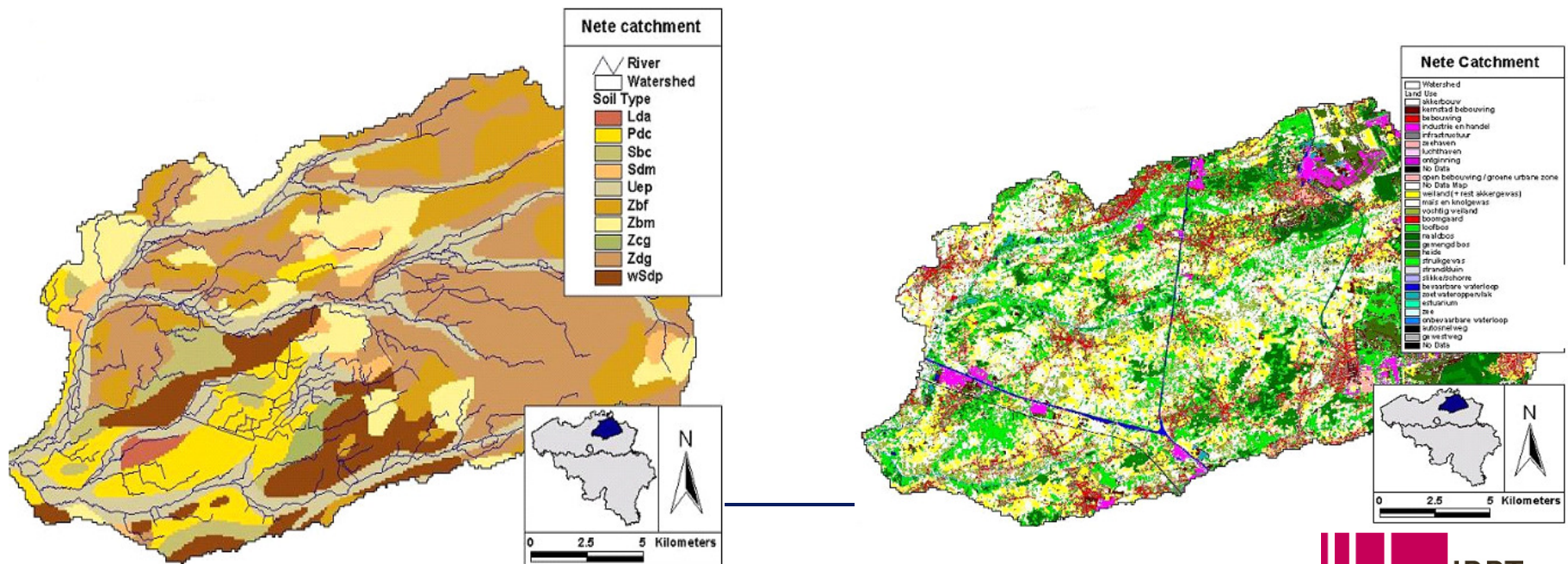
■ David data

- (From the Digital Michelangelo project, Stanford University)



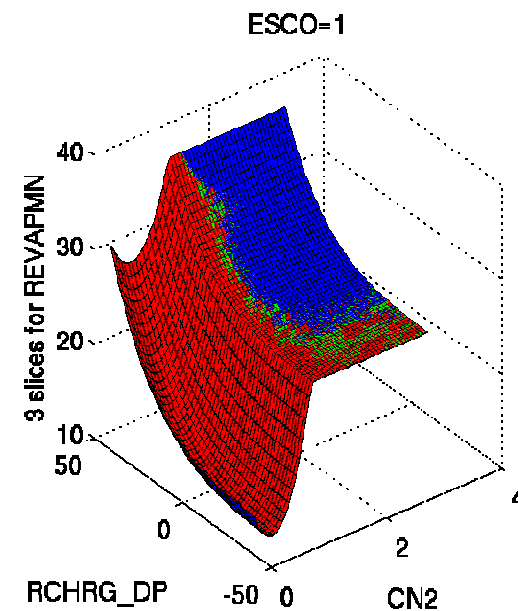
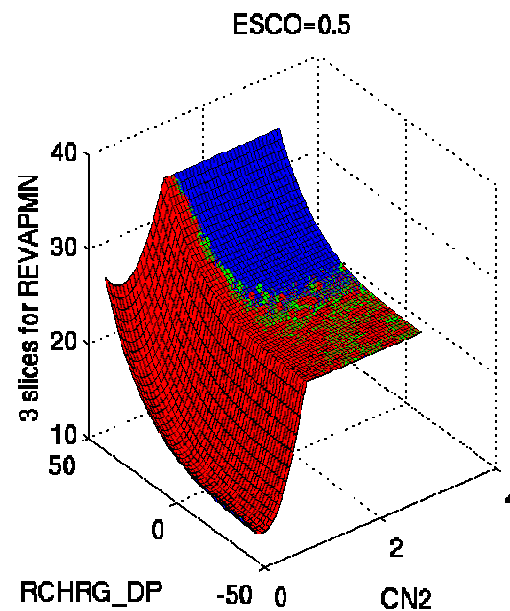
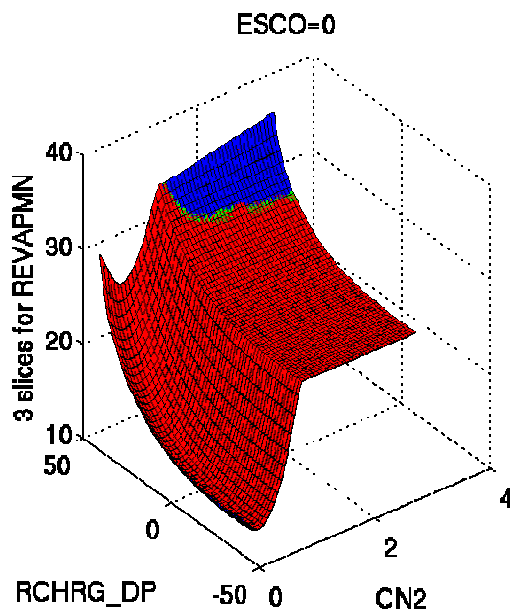
■ Soil and Water Assessment Tool

- river basin model (Grote Nete, Belgium)
 - ◆ **Quantify the impact of land management practices in large, complex watersheds**
 - Runtime for one simulation: 4 to 10 minutes
- **SWAT2005:** <http://www.brc.tamus.edu/swat/>



■ Approximating global behaviour

- Models error (MSE) between SWAT and observations
- Constructed model with 1016 samples
 - ♦ 5.6 samples in each dimension (4 dimensions)
 - ♦ 3.1 percent error (generating validation set on-the-fly)

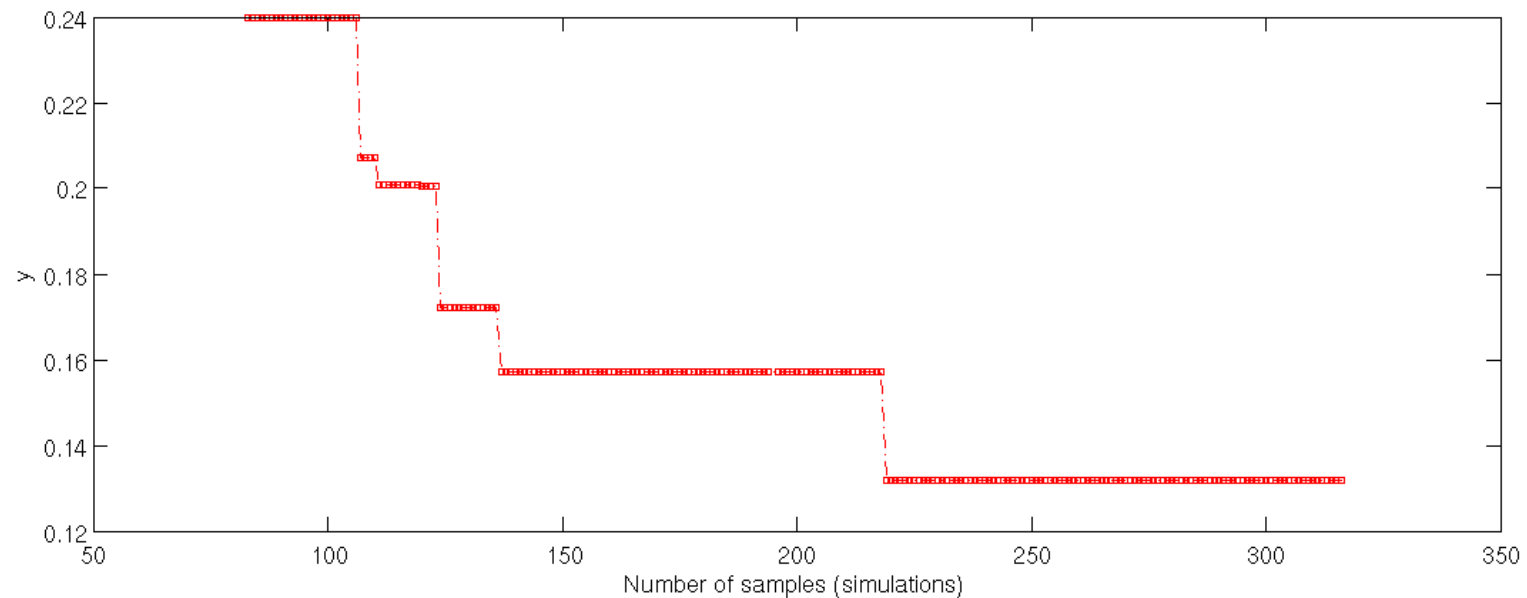


- **Band-pass filter (2.32-2.56 Ghz)**
- **Software: MicroWave Studio (MWS)**
 - Computer Simulation Technology (CST)
- **Inputs: 5 dimensions**
 - Spacing: S1, S2
 - Offsets: Off1, Off2, Off3
- **Output**
 - Max(S-parameter) between 2.32 and 2.56 Ghz
- **Simulation time: 5 – 10 minutes**
- **Optimization algorithm: EGO + Kriging**

■ Initial design of 83 samples

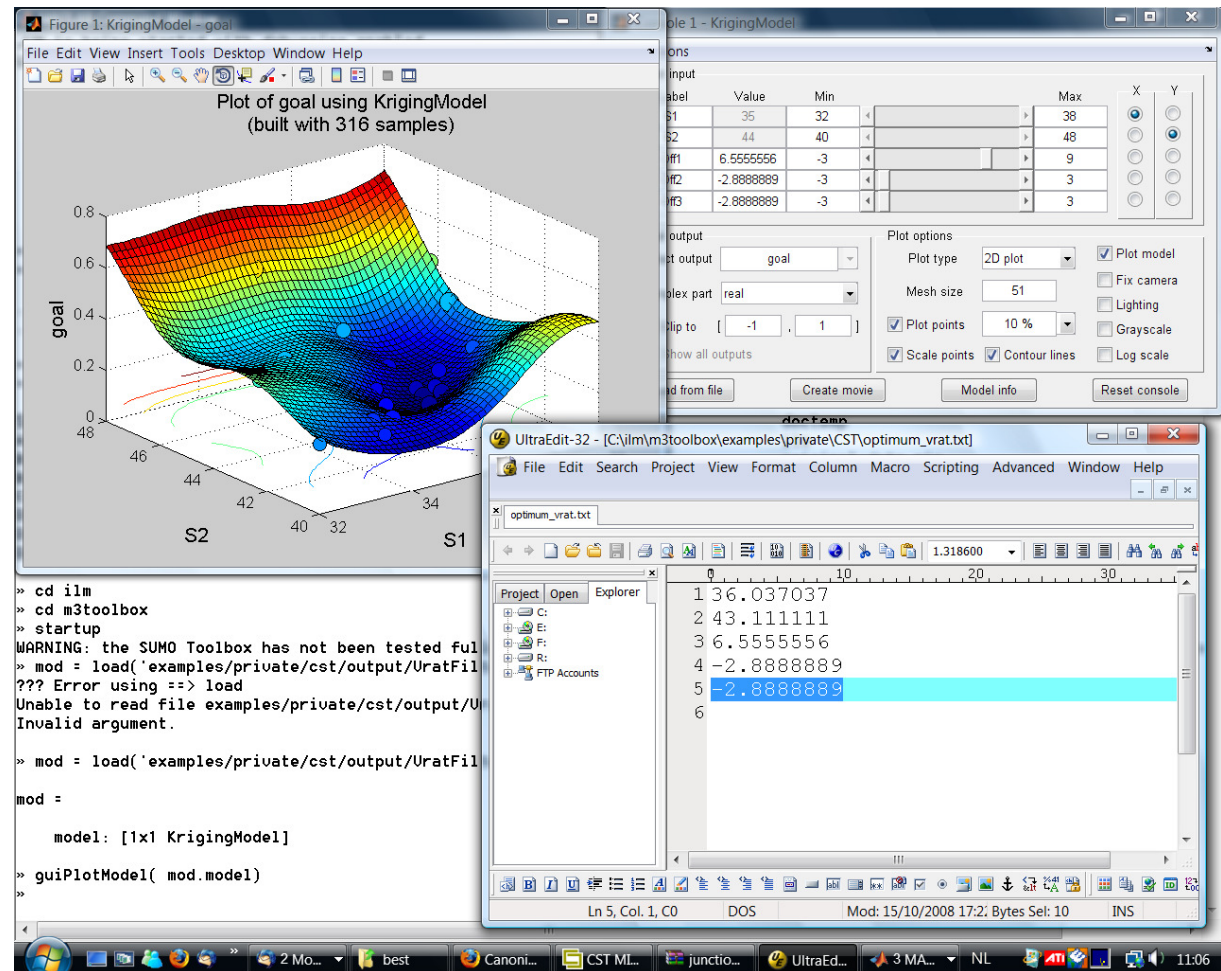
■ Results

- 'Very good' minimum after ~150 samples
- Add 100 simulations more 'to be sure'



■ Model browser

- Sensitivity
- Robustness
- ...

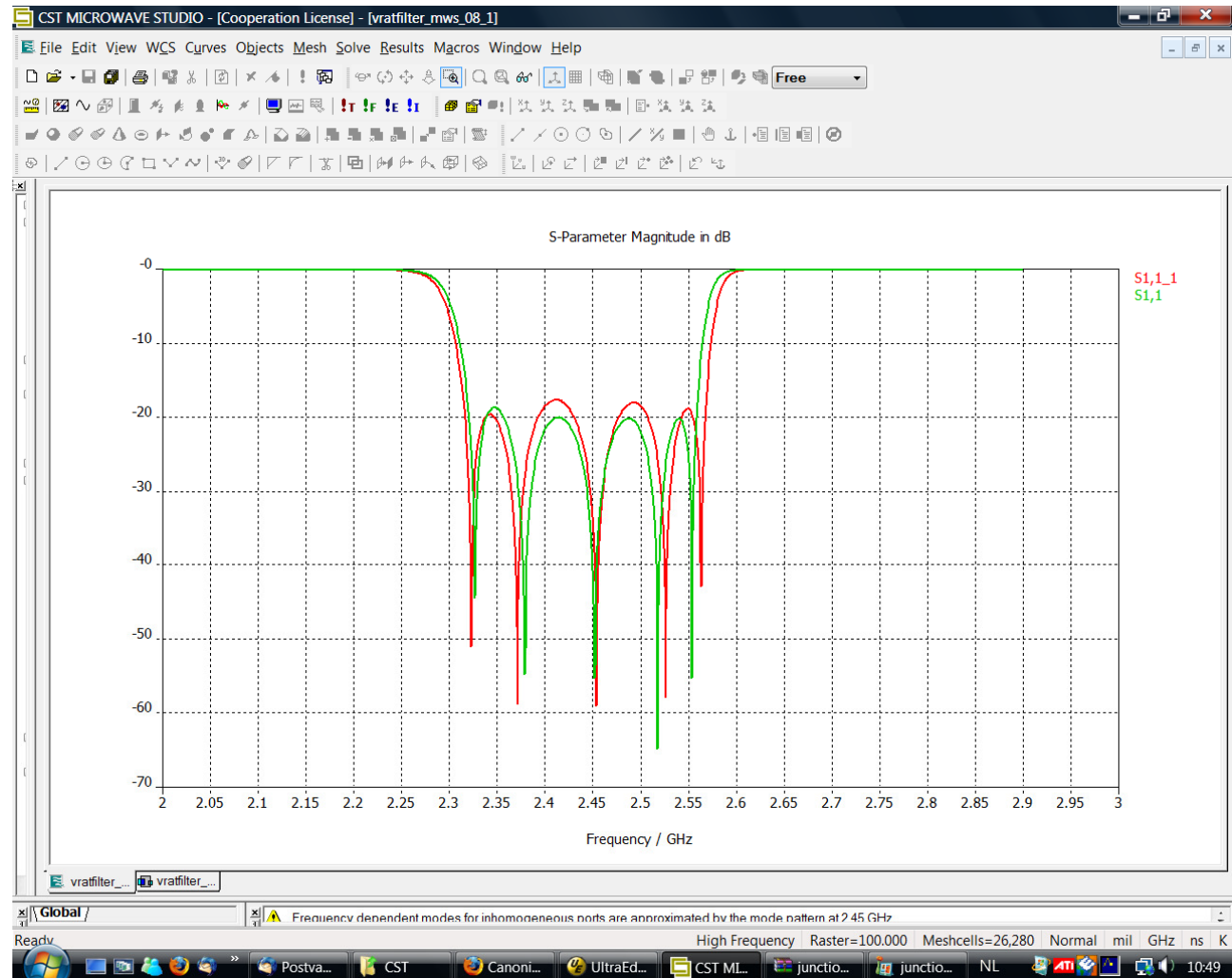


■ Green curve

- Reference

■ Red curve

- Optimum found



- Who are we ?
- Introduction
- Surrogate modeling
- SUMO Toolbox
- Examples
- Conclusions

■ Compact surrogate models

- Global, local

■ Fully automated

- Adaptive model selection
- Adaptive sample selection
- Distributed computing
- (optimization)

■ Surrogate Modeling (SUMO) Toolbox

- Easy to setup and run different modeling experiments
- Natural platform for benchmarking different techniques
- Download from <http://www.sumo.intec.ugent.be>



Thank
You

■ Questions ?